The Thesis Committee for Talal Eid Alotaibi
Certifies that this is the approved version of the following thesis:

Examination of Focal Adhesion Kinase's FAT Domain Structural Response to Applied Mechanical Load

APPROVED BY

SUPERVISING COMMITTEE:

Tess J. Moon, Supervisor

Pengyu Ren

Examination of Focal Adhesion Kinase's FAT Domain Structural Response to Applied Mechanical Load

by

Talal Eid Alotaibi, B.E

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Dedication

Dedicated to my mother Modhi

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Abstract

Examination of Focal Adhesion Kinase's FAT Domain Structural Response to Applied Mechanical Load

Talal Eid Alotaibi, M.S.E

The University of Texas at Austin, 2012

Supervisor: Tess J. Moon

Focal adhesion kinase (FAK) is a non-receptor tyrosine kinase. Activated FAK is crucial to many biological processes, such as cell proliferation, migration, and survival, all of which have been implicated in the progression and development of cancer. Tyrosine 925 is a Src-phosphorylation site that is located within the FAT domain in the C-terminal of FAK. It has been suggested that the helix containing Y925 (Helix 1) has to come out of the FAT bundle and the region flanking Y925 has to adopt β-strand conformation. In order to phosphorylate, the mechanisms promoting the required structural changes are unclear. So, Molecular Dynamics (MD) and Constant Force Molecular Dynamics (CFMD) simulations were used to study what makes Y925 accessible for phosphorylation.

Under thermal fluctuation only and in the presence or the absence of LD motifs, MD simulations suggest that H1 does not appear to have a propensity to leave the bundle adopt β-strand conformation. Then, two different load scenarios were used; axial and perpendicular with 100 pN constant load applied to H1 N-terminus with the two paxillin

LD motifs constrained. For both load scenarios, H1 has two different behaviors: typical and atypical. In the axial load scenario, the first two residues at the N-terminal of H1 (besides Y925) have low propensity to unfold. However, H1 does not show any proclivity to leave the bundle. For the perpendicular load scenario with the absence of P2 (LD motif binds to H1/H4 hydrophobic patch), one simulation out of 21 showed that H1 undergoes the required structural rearrangement. In general, CFMD simulations show that the FAT domain has a very low propensity (3%) to undergo the structural changes needed for Y925 phosphorylation. This has two implications: either mechanical load is insufficient to make Y925 available for phosphorylation and/or this kind of process (structural changes needed for Y925 phosphorylation) is slow process that needs a long time to occur.

Table of Contents

List of Tables

List of Figures

Chapter 1. Introduction

1.1 Focal Adhesion Kinase (FAK)

Focal adhesion kinase (FAK), a non-receptor tyrosine kinase regulated by integrins and expressed in most cell types, plays an important role in signal transduction [1]. Activated FAK is crucial to many biological processes, such as cell proliferation, migration, and survival. These processes are involved in the progression and development of cancer, in which an increased FAK signal might result in one these biological processes being uncontrolled [2].

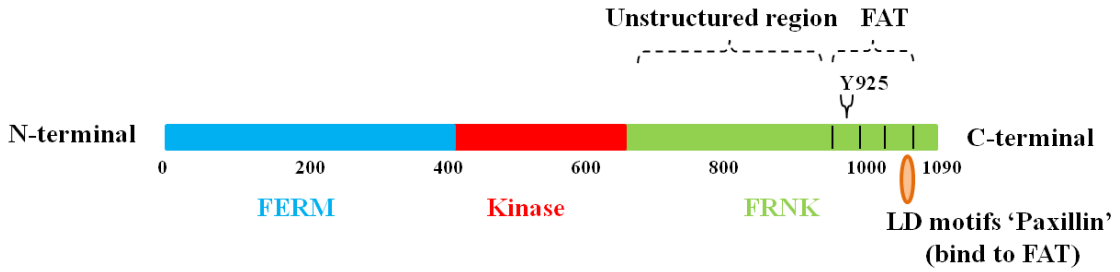


Figure 1-1: The organization of FAK, which starts with a non-catalytic FERM domain located at the N-terminal; a catalytic kinase domain in the mid section; and a non-catalytic FRNK domain at the C-terminal. The FRNK domain consists of two domains: the unstructured region and FAT domain (modified [1])

In a number of tumors, including those seen in breast and prostate cancer, the expression of FAK is elevated. Furthermore, experimental overexpression of FAK in cells can increase the growth of cancer cells and invasion. Clinical evidence suggests an important role of FAK in the formation and progression of tumors [3].

The importance of FAK in cell function and the progression and development of cancer suggests the importance of FAK as a potential target for cancer therapy. Inhibition or control of FAK may show promise as a cancer treatment [2].

FAK has multiple domains, which starts with a non-catalytic FERM domain located at the N-terminal; a catalytic kinase domain in the mid section; and a non-catalytic FRNK domain at the C-terminal. The FRNK domain consists of an unstructured region at its N-terminal and FAT (Focal Adhesion Targeting) domain at the C-terminus [1].

1.2 Focal Adhesion Targeting Domain (FAT)

The FAT domain, which consists of four anti-parallel helices bundled together, has a critical phosphorylation site Y925 that has been implicated in cancer growth [4]. Phosphorylation of this site by Src-kinase family promotes the dissociation of FAK from focal adhesions and creates a binding site to the Grb2-SH2 domain.

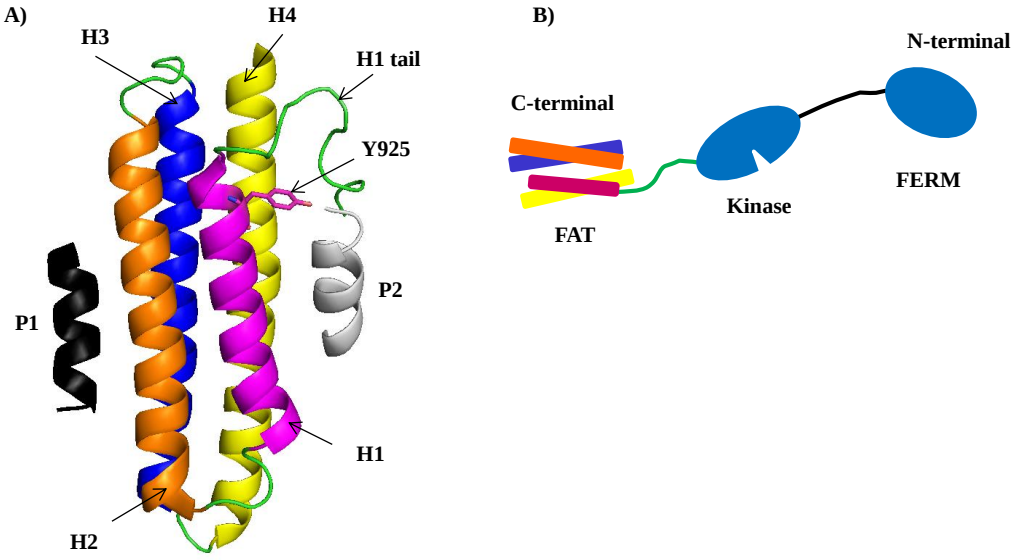


Figure 1-2: The structure and location of Focal Adhesion Targeting (FAT) domain. A) Cartoon representation of the FAT/paxillin complex. The construction of this complex is described in detail in chapter 3 (Methodology, Structures, Figure 3-1). The first helix (H1) of this complex is shown in magenta, the second helix (H2) in orange, the third helix (H3) in blue, and the last helix (H4) in yellow. The paxillin LD motifs are represented as follows: LD4, that binds to the first hydrophobic patch HP1, is shown in black (named P1), LD2, that binds to the second hydrophobic patch HP2, is in white (named P2). P1 and P2 will be used in this thesis. B) Illustration of the location of the FAT domain relative to the Kinase and FERM domains.

One phosphorylation site of FAT is Y925, which is located near the N-terminal of the FAT domain. Several hypotheses suggest that conformational changes must take place for this site to be phosphorylated; the actual mechanism is unclear. However, since the phosphorylation of this site is critical, it is important to have a better understanding of what is required of make this site available for phosphorylation. In addition to subjecting this site to thorough investigation, useful insight could be gained and how to create inhibitions preventing its phosphorylation.

1.3 Y925 Phosphorylation Requirements

The closed-bundle form of the FAT domain is sufficient to create two binding affinities via the two hydrophobic patches to which paxillin and other scaffolding proteins bind. The FAT domain in its bundled form is a poor substrate for Src-kinase so H1 that carries Y925 has to come out of the bundle [5]. In addition, the region of Y925 has to adopt β-strand conformation to engage the phosphorylation by Src-kinase [6]. Moreover, the Grb2-SH2 domain cannot bind to phosphotyrosine residues unless the area flanking it also adopts β-strand conformation [5] (Figure 1-3). All these requirements for phosphorylation, along with their references, are presented in the literature review.

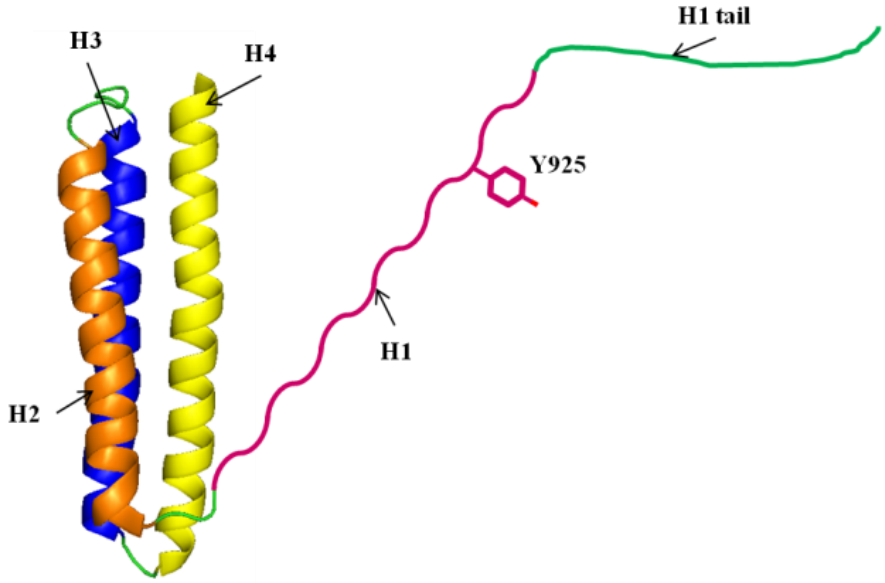


Figure 1-3: The hypothesized structure of the FAT domain that is required for Y925 phosphorylation. H1 comes out of the bundle as well as the region flanking Y925 adopts a β-strand conformation.

1.4 Understanding Pre-Phosphorylation Process

The previously described requirements for phosphorylation do not demonstrate what makes these structural changes occur; therefore, thorough investigation of this

process is essential to its understanding. Specifically, because it has been suggested that the first helix (H1), which contains Y925, is strongly attached to the bundle, the mechanism by which that energy barrier is overcome to get H1 out of the bundle must be ascertained. To accomplish this goal, which is to understand the mechanism that occurs before phosphorylation, one needs to go look deeply into the FAK environment.

FAK is presumably mechanically activated through extracellular matrix (ECM) proteins and actin cytoskeleton contractility [7-9]. The mechanical activation can be simply performed by molecular stretch, in which the N-terminal of FAK, the FERM/ligand complex, is mechanically pulled to disrupt the complex. This results both in release of auto-inhibition and activation of FAK (Figure 1-4) [10].

Two tethers are required for the existence of this mechanism. The N-terminal of FAK is suggested to be a tether, in which the FERM domain interacts with basic patch ligand [11]. On the other C-terminal side of the FAK , the FAT domain binds to paxillin and creates the opposite tether. Focusing on the FAT/paxillin complex, the load comes from the rest of the FAK through H1, while the LD motifs are considered reactions.

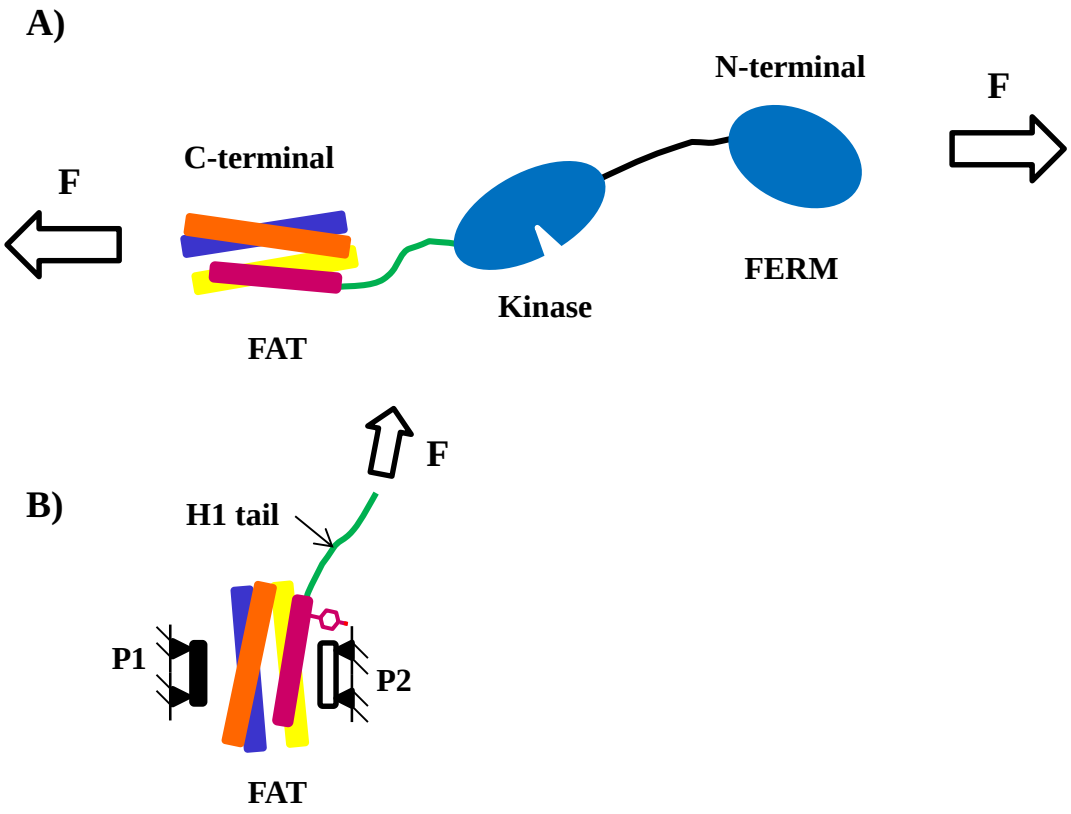


Figure 1-4: The hypothesized mechanism of the activation of the FAK. A) The N-terminal of the FAK (FERM domain) acts as a tether while the C-terminal (FAT domain) acts as an opposite tether. When loaded at both terminals, FAK is presumably mechanically activated. B) The hypothesized activation mechanism of FAT domain where the load comes from the rest of FAK through H1 tail and LD motifs (P1, P2) act as reactions.

Computational program were used to achieve this goal. Molecular Dynamic Simulation programs, (GROMACS: GROningen MAchine for Chemical Simulations, CHARMM: Chemistry at HARvard Molecular Mechanics, and others), are able to facilitate an acceptable imitation of the environment in which the protein lives. Specifically, GROMACS, was used, to run Molecular Dynamics (MD) simulations as well as Constant Force Molecular Dynamics (CFMD) simulations. MD is used to look at the protein's behavior at equilibrium, while CFMD is performed to examine the effect of the applied load on the behavior of the protein.

For the FAT domain, it is essential to understand both its mechanical behavior and its propensity to undergo the necessary structural changes required for phosphorylation at equilibrium. Then, CFMD is used to apply the load to the FAT domain in a location and direction thought physiologically reasonable to induce the required conformational changes.

The following chapter includes a detailed review of the literature on the FAT domain, including what is known about the structure, binding affinities, binding partner, and phosphorylation site of the FAT domain, as well as the rationale behind the hypotheses suggesting the requirements needed for phosphorylating the FAT domain.

Methodology follows the literature review and includes a full description of how the FAT/paxillin complex is constructed. In addition, it includes the cases and simulations that must be run for both the equilibrium and loading cases. It also contains an illustration of how a certain hypothesis can be statistically addressed, such as the position of the first helix relative to the bundle, as well as the unfolding of the residues flanking Y925.

The Results section includes a discussion of the matrices chosen. It is divided into two main sections: the equilibrium results and the mechanical loaded results. Connecting the statistical results with the biological implications is the main goal of this chapter.

Finally, Conclusions gives an overall discussion of the results, including what may be required to accomplish the phosphorylation process. It also raises questions that are important to address in future research.

Chapter 2. Literature Review

2.1 Focal Adhesion Kinase (FAK)

FAK, which is 1,090 residues long, consists of a catalytic kinase domain flanked by two non-catalytic domains, the FERM domain (erythrocyte band 4.1 ezrin-radixin-moesin) located in the N-terminus and the C-terminal domain or FRNK (FAK-related-non-kinase) domain (Figure 1-2). The FRNK domain consists of two domains: the unstructured region at the N-terminal and FAT domain (Focal Adhesion Targeting) at the C-terminal [1].

2.2 Focal Adhesion Targeting (FAT) Domain

FAT is approximately 140 amino acids long and is located at the C-terminus of FAK. The importance of the FAT domain comes from the fact that it is sufficient for localizing and targeting FAK to focal-adhesion-associated proteins such as paxillin and talin [12-14]. Even Y925 (within FAT) is not a typical phosphorylation site in vivo [15]; the phosphorylation of this site has been implicated in cancer growth [4], an important topic of further investigation (Y925 in human, mouse sequences and Y926 in avian sequence).

2.2.1 FAT STRUCTURE

The FAT domain is an antiparallel, “right-handed” four-helix bundle with short loops that is maintained by hydrophobic interactions [13]. It has been shown that the

hydrophobic core of the FAT domain is well defined and highly conserved across species. The first helix, H1, is the shortest one, while the fourth helix, H4, is the longest one (Figure 1-2). The H1 helix of the FAT domain contains Y925 tyrosine which is located at the start of the second turn of H1 and is phosphorylated by Src-kinase family [15].

The analysis of the FAT domain surface has shown that FAT has two hydrophobic-patch binding sites, HP1 at the H2H3 face and HP2 at H1H4 on the opposite side, where the FAT domain binds to paxillin via its two helical LD motifs (Figure 1-2, the white and black helices). A short loop, which contains two proline residues, is between H1 and H2 and is identified as a hinge region because of its flexibility [12, 16].

2.3 Paxillin

Paxillin is an adapter, focal adhesion-associated protein that targets a number of proteins to the focal adhesions and is believed to be responsible for gathering multi-protein complexes to a coordinate signaling [17]. Paxillin is presumed to be a regulator for cell spreading and motility. The N-terminal of paxillin, an unstructured protein, contains a proline-rich region and five copies of approximately 13 peptide residues called LD (leucine-aspartate) repeat motifs, which form amphipathic α-helices. LD motifs are known to be binding sites for proteins such as FAK, vinculin, and others [18]. The C-terminal of paxillin contains four LIM domains, which are responsible for targeting the paxillin to the focal adhesions [19].

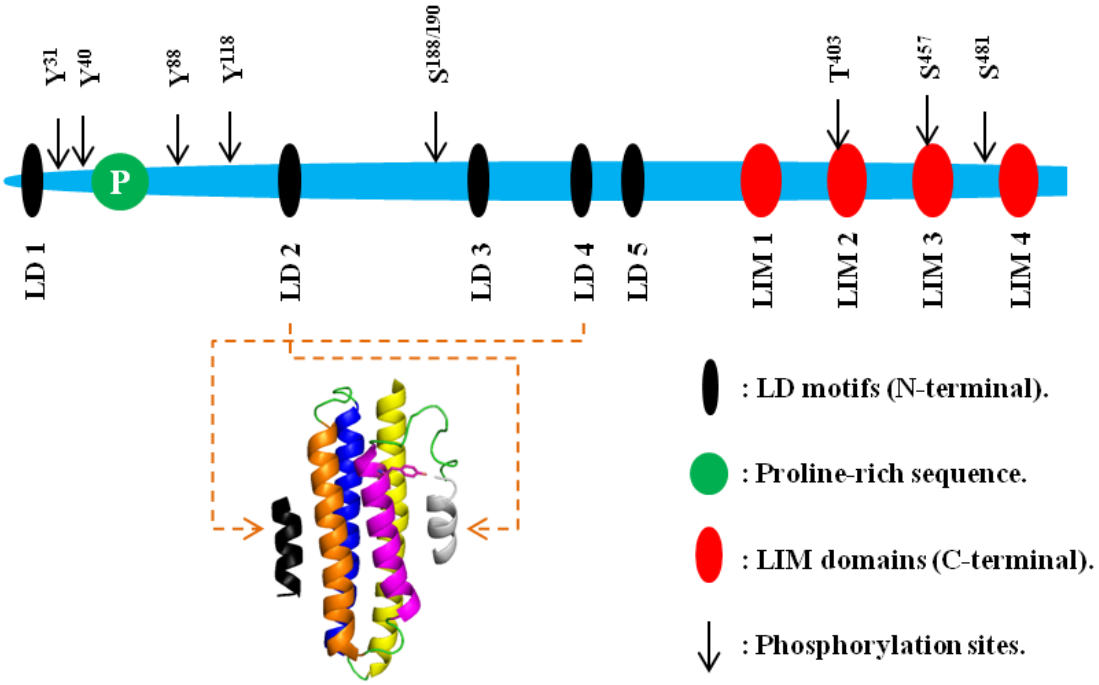


Figure 2-1: An organization of the different domains of paxillin, including the two LD motifs that bind to the FAT domain (LD4 'P1' at HP1 and LD2 'P2' at HP2) (modified [17]).

2.4 Paxillin Association with FAT

The localization of FAK to the focal adhesions is performed by binding to the paxillin. The two hydrophobic patches HP1 and HP2 of the FAT domain of FAK are the binding sites of the two LD motifs: LD4 (P1) binds to HP1 at H2H3, and LD2 (P2) binds to HP2 at H1H4, near where Y925 is located (For the entire thesis, LD motifs will be called as follows: LD4 'P1' and LD2 'P2'). The closed-conformation, bundled form of the FAT domain is presumed to be important for FAT to bind to paxillin [20]. Disrupting these interactions between LD motifs and FAT is likely to break down the localization of FAK. On the C-terminal of paxillin [17], the third LIM domain has a major role in targeting the paxillin to the focal adhesions [19]. In addition, the association of paxillin with FAK or other kinases, such as Src, has an important role in controlling and

promoting the tyrosine phosphorylation of paxillin, which is involved in cell spreading and motility [10].

2.5 Phosphorylation of Y925

Located in the second turn of H1 of the FAT domain, Y925 is known to be the phosphorylation site by Src family tyrosine kinases. Phosphorylation of Y925 creates a binding site of FAT to Grb2-SH2. This provides a mechanism of activation of the ras/MAPK pathway [15]. As a results of Y925 phosphorylation of the FAT domain, FAT is presumed to dissociate from the paxillin, leading to dissociation of FAK from the focal adhesions [20]. The mechanism by which Y925 is phosphorylated and what is required for Y925 to bind FAT to Grb2-SH2 remains unclear.

Experimental results suggest that FAT has to undergo some structural rearrangement, such that Y925 is pointed toward the Src kinase-active site to be phosphorylated [5]. The requirements for creation of access of the Src kinase and Grb2-SH2 to the Y925 phosphorylation site are illustrated below:

2.5.1 H1 Position

The unphosphorylated FAT domain is a poor substrate for tyrosine kinases in its bundled, or closed-conformation, form [5]. Therefore, some structural rearrangement of the FAT domain are hypothesized to take place in order to make FAT a tyrosine kinase substrate. Another structure of the FAT domain, called a swapped dimer [5, 21] (Figure 2-2), in which each of the two FAT domains exchanges its first helix, has been observed in vitro. Even the infrequent appearance of this type of structure, “which has grown, *in*

vitro, in six months comparing it with bundle form that has grown in three weeks," suggests that H1 has capacity to leave the bundle. Other researchers have suggested that during the formation of the swapped dimer that there will be a transition state in which H1 is less structured. During the transition state, the region around Y925 could adopt the required structure and engage the phosphorylation [20] (Figure 1-3).

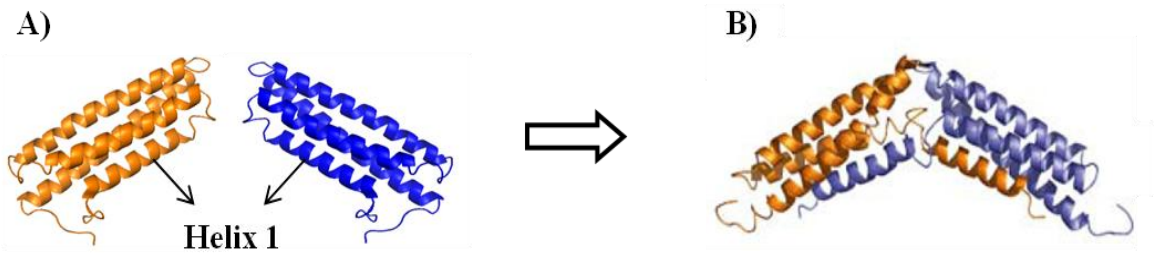


Figure 2-2*:* Illustration of an observed swapped dimer created in vitro after six months in solution. A) Two different FAT domains in a four-helix bundle form. B) The swapped dimer structure is formed when two FAT domains exchange their first helix (modified [21]).

In addition, it has been reported that the Vinculin tail, "Vt" [22] and apolipoprotein E 'apoE' [23], which have close structural similarities to FAT, undergo a functional folding/unfolding transition [5] (Figure 2-3). The unusual arrangement of the FAT helices and P944XPP peptide "short loop that connects H1 and H2" might enable such transitions [5, 20]

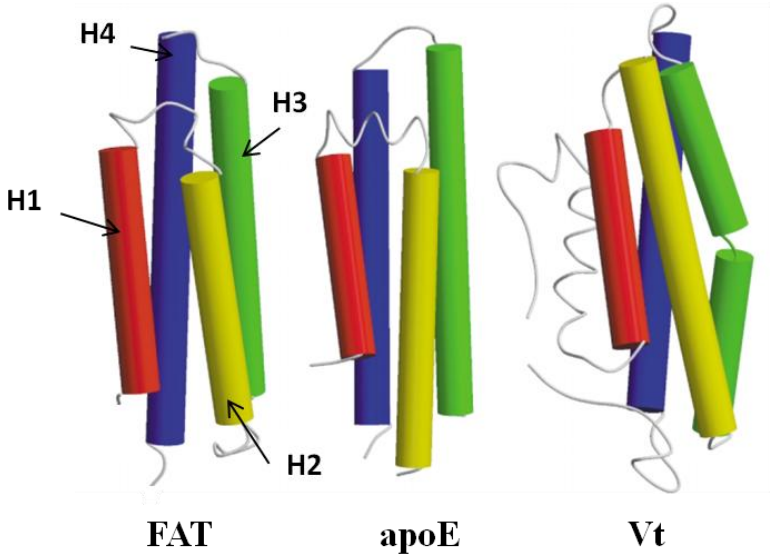


Figure 2-3: FAT domain, including two structural homologues apolipoprotein E (apoE) and the Vinculin tail (Vt) (modified [13]).

As a result, it has been suggested that FAT's H1 must be in an open conformation, specifically with H1 out of the bundle, in order for FAT to engage the phosphorylation [20]. Since H1 is part of the bundle in native form, this means that it has to overcome an energy barrier, by undergoing some unfavorable conformational changes, in order to open out.

2.5.2 H1 UNFOLDING

The Src-like tyrosine kinases can bind to a tyrosine located in a region that adopts β-strand structure [6]. In addition, it is known that Grb2-SH2 binds to phospho-tyrosine that is within a β-strand region [24]. The helical conformation of H1 hinders any interaction between Y925 and Grb-SH2 unless it adopts β-stand conformation. This suggests that the phosphorylation of the FAT domain requires that the region flanking Y925 has to be in a β-strand conformation [5] (Figure 1-3).

2.6 Salt Bridges between H1 Tail and H4

Based on the published crystal structures, there are two salt bridges, among other factors, contributing to an energy barrier preventing H1 to open out (Figure 2-4). Those salt bridge interactions are between the extensional loop of H1 (for this thesis, called the H1 tail) and H4 which have been observed from the crystal structure [5]. The first salt bridge, 'SB1', is between H1 tail R919 and H4 D1039. The second one, 'SB2', is between H1 tail D922 and H4 R1042.

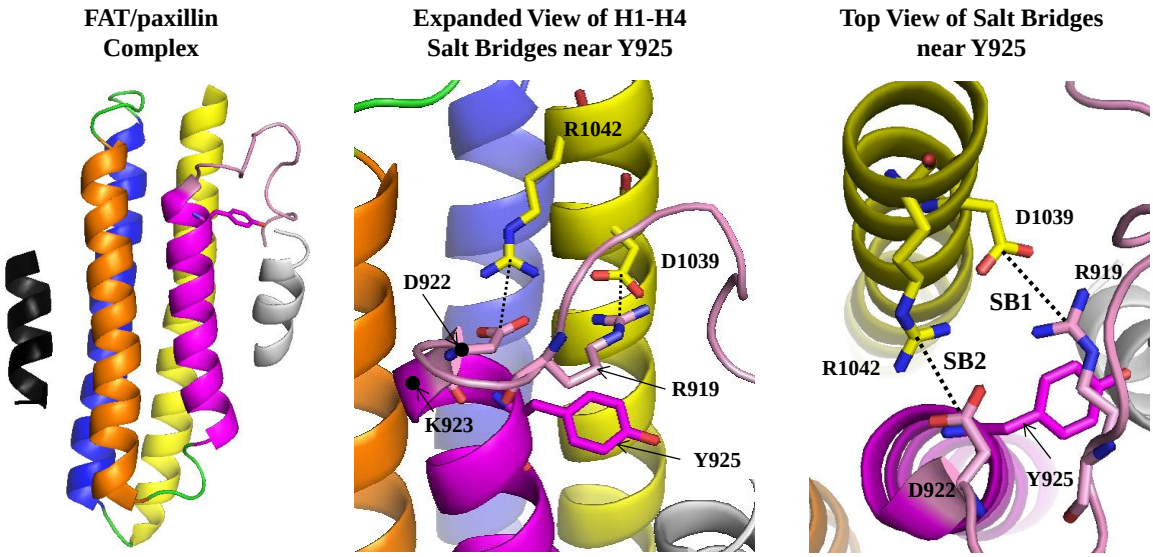


Figure 2-4: Two salt bridges that are located in the region near the N-terminal of H1 (near Y925). Those salt bridges are between H1 tail and H4 (SB1: R919-D1039 and SB2: D922-R1042).

2.7 Methionine Zipper between H1, H2, H3 and H4

The "bottom" of the FAT domain (near the C-terminal of H1) involves an obvious cavity form by a hydrophobic cluster consisting of four hydrophobic residues, methionines, which disrupt the packing of the hydrophobic core of the FAT domain

(Figure 2-5) [5, 12]. Since these residues are far away from Y925, it is presumed that they do not have a significant influence of the mechanical behavior region flanking Y925.

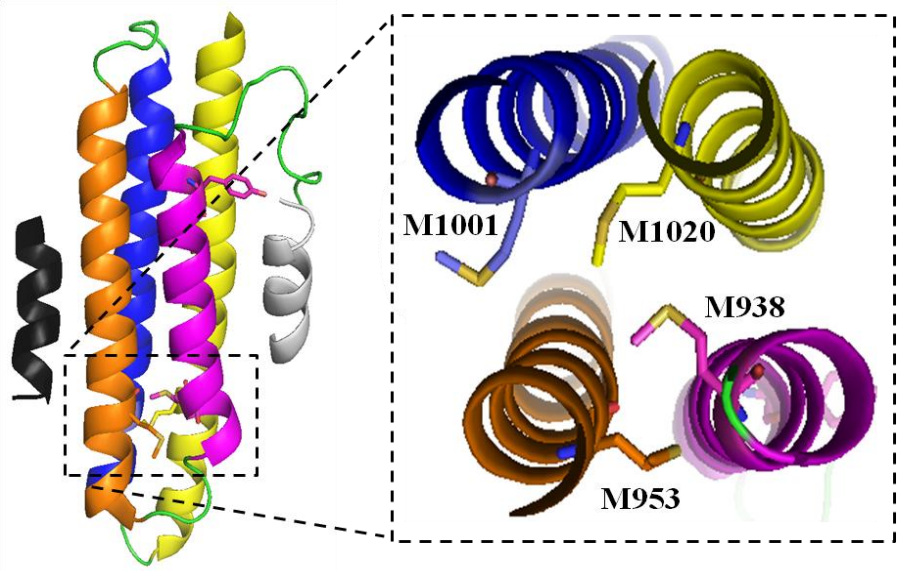


Figure 2-5: Methionine zipper is formed by four methionine residues, one each from the form helices. The view shown is roughly along the bundle's central axis near region of the C-terminal of H1 where those methionine residues located.

2.8 Interactions between Paxillin LD Motifs and FAT Domain

Some interactions between FAT and LD motifs may be important in maintaining the association of FAT domain and paxillin. The aspartic acid from P1, D146, interacts with R962 and/or K955 from H2. Another aspartic acid, D268, from P2 interacts with either H1025 and/or K1032 from H4 [12] (Figure 2-6). Since the main goal of this research is to examine the availability of Y925 for the physphorylation, the strength of these interactions are not examined.

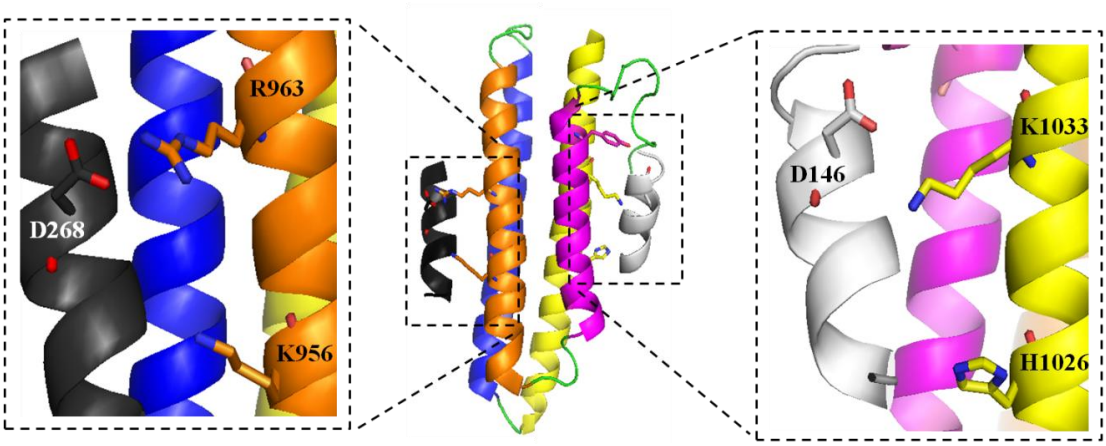


Figure 2-6: Electrostatic interactions between paxillin and the FAT sub-domain. The left figure shows the interactions between P1 and H2, while the right figure illustrates the interaction between P2 with H4.

Table 2-1: A summary of the reported interactions of the FAT/paxillin complex. Salt bridges are shown in red, methionine zipper is in green and electrostatic interactions are in blue.

	P1	P2	H1	H2	H3	H4
H1			M938 [5, 12]			H1: R919 - H4: D1039 [5] H1: D922 - H4: R1042 [5]
H2	P1: D268 H2: R963 & K956 [12]			M953 [5, 12]		
H3					M1001 [5, 12]	
H4		P2: D146 H4: H1026 & K1033 [12]				M1020 [5, 12]

Chapter 3. Methodology

To understand the FAT domain's mechanical behavior and examine the availability of Y925 for the phosphorylation, (MD) and Constant Force Molecular Dynamics (CFMD) simulations of FAT/paxillin complex were run using GROMACS [25, 26] and analyzed using scripts written the MATLAB programming language. The methodology chapter has three main sections: Structures, Simulations and Analysis. The structure section illustrates how the structures that are used in the simulation were constructed. The simulation section presents a description of all type of simulations that are run. The analysis section includes all the analysis used for investigating the FAT domain behavior, including the behavior of H1 that contains Y925.

3.1 Structures

The FAT/paxillin complex has been constructed and modified in order to be used in the equilibrium MD and loaded CFMD simulations.

3.1.1 FAT/PAXILLIN COMPLEX WITHOUT H4 TAIL AND P1/P2 UNCONSTRAINED

The FAT/paxillin complex that is shown in Figure 1-2 was built through these steps:

1. A crystal structure of FAT/LD4 motif complexes (PDB entry 1ow7) [27] was downloaded from the Protein Bank Database (www.pdb.org). This PDB file includes multiple FAT domains that bind to LD4 motifs from either binding site. As seen in Figure 3-1.A, in the first complex from the left, the LD4 motif (chain D in yellow) binds to the FAT domain (chain A in green) at the second

hydrophobic patch HP2 (between H1/H4). In the second complex, the LD4 motif (chain E in grey) binds to the FAT domain (chain B in magenta) at the first hydrophobic patch HP1 (between H2/H3). The third complex consists of the LD4 motif (chain F in dark pink) binds to the FAT domain (chain C in cyan) at the first hydrophobic patch HP1 (between H2/H3).

2. Using Pymol (Molecular Visualization Program: http://www.pymol.org/), the two FAT domains that bind to LD4 motifs (first and third complexes) were selected for alignment.
3. Pymol has options for aligning two molecules. In one option, Pymol minimizes the RSMD (Root Mean Square Deviation; the square root of the mean of the square of the distances between aligned atoms) between aligned molecules. For this study, the backbone atoms of the two selected FAT domains (chain A: N916-T1049 and chain C: I909-G1047) were aligned based on minimizing the RMSD forming the two overlapped FAT domains that bind to LD motifs from two hydrophobic patches shown in Figure 3-1.B.
4. One FAT domain (chain C) and the two LD4 motifs (chain D and chain F) were retained forming the final FAT/paxillin complex as shown in Figure 3-1.C.

The final FAT/paxillin structure with the presence/absence of P1 and P2 was used in all equilibrium simulations (Table 3-1: EQ.WOT.P1P2, EQ.WOT. P2, EQ.WOT.P1 and EQ.WOT.Ø). Detailed descriptions of the cases that are considered for the equilibrium simulations are presented in §0Simulations.

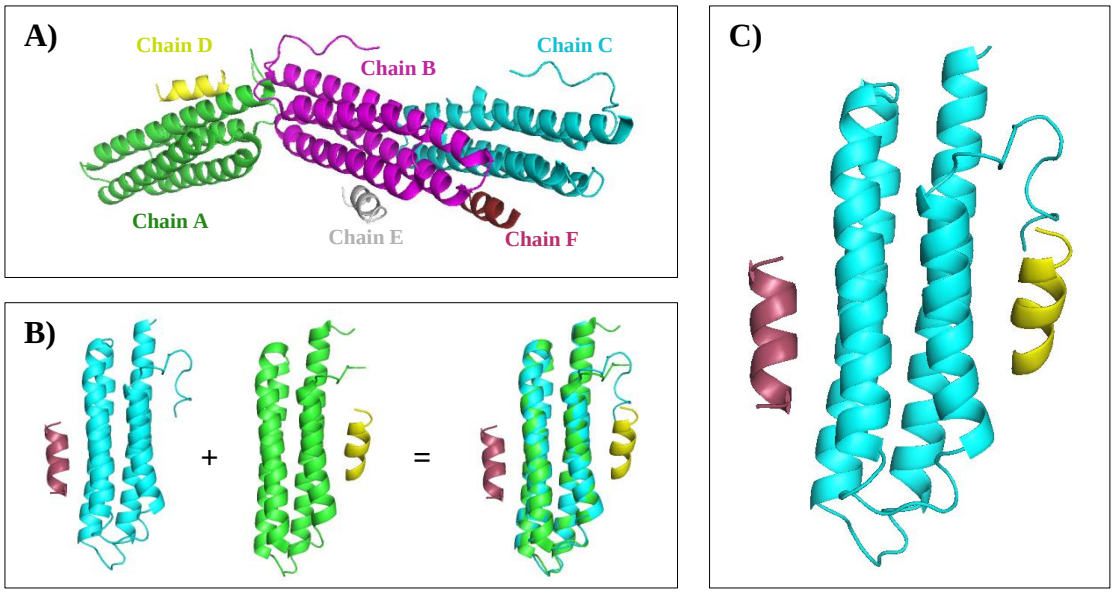


Figure 3-1: FAT/paxillin complex without H4 tail and P1/P2 unconstrained. A) Three different FAT domains (green, magenta and cyan) that bind to the LD motifs (yellow, grey and dark pink) from either side. B) Selected FAT domains (FAT domain binds to LD motif at HP2 and FAT domain binds to LD motif at HP1) from pdb entry 1ow7 and the overlapped structure. C) FAT/paxillin complex. This structure was used for equilibrium (EQ) without H4 tail (WOT) simulation (Table 3-1).

3.1.2 AUGMENTED FAT/PAXILLIN COMPLEX WITH H4 TAIL AND P1/P2 CONSTRAINED

The FAT/paxillin complex (Figure 3-1.C) was modified for the loaded simulations. As it has been suggested that FAK is mechanically activated, this research investigated mechanically loaded cases using Constant Force Molecular Dynamics (CFMD) simulations. Constant mechanical loads were applied at the N-terminus of H1 (I909) in directions parallel and perpendicular to the H1 axis. The load must be applied to the extensional loop at the FAT domain's N-terminal of that connects the FAT domain with the rest of the FAK domain, the presumptive origin of the mechanical load . In addition, since the paxillin associates the FAT domain to the focal adhesions, the LD motifs to which FAT binds are presumed to act as tethers. However, the key step is to make the load scenarios as realistic as possible before starting any simulations.

3.1.2.1 H4 Tail Addition

Random-coil residues missing from the crystal structure must be added to pdb structure at the C-terminal of the FAT domain, where they belong.

1. Using “builder” command in Pymol, the five residues missing from the pdb (QTRPH) were added to the C-terminal of residue G1047 based on the FAK sequence (Figure 3-2, Figure 3-4).
2. Since the structure of those residues is unknown, their initial structure is assumed to be random coil. The results are not expected to be sensitive to this initial placement as this coil will move in such a way that it finds its natural position after the energy minimization and equilibration processes. This extensional loop is named H4 tail over the entire thesis.

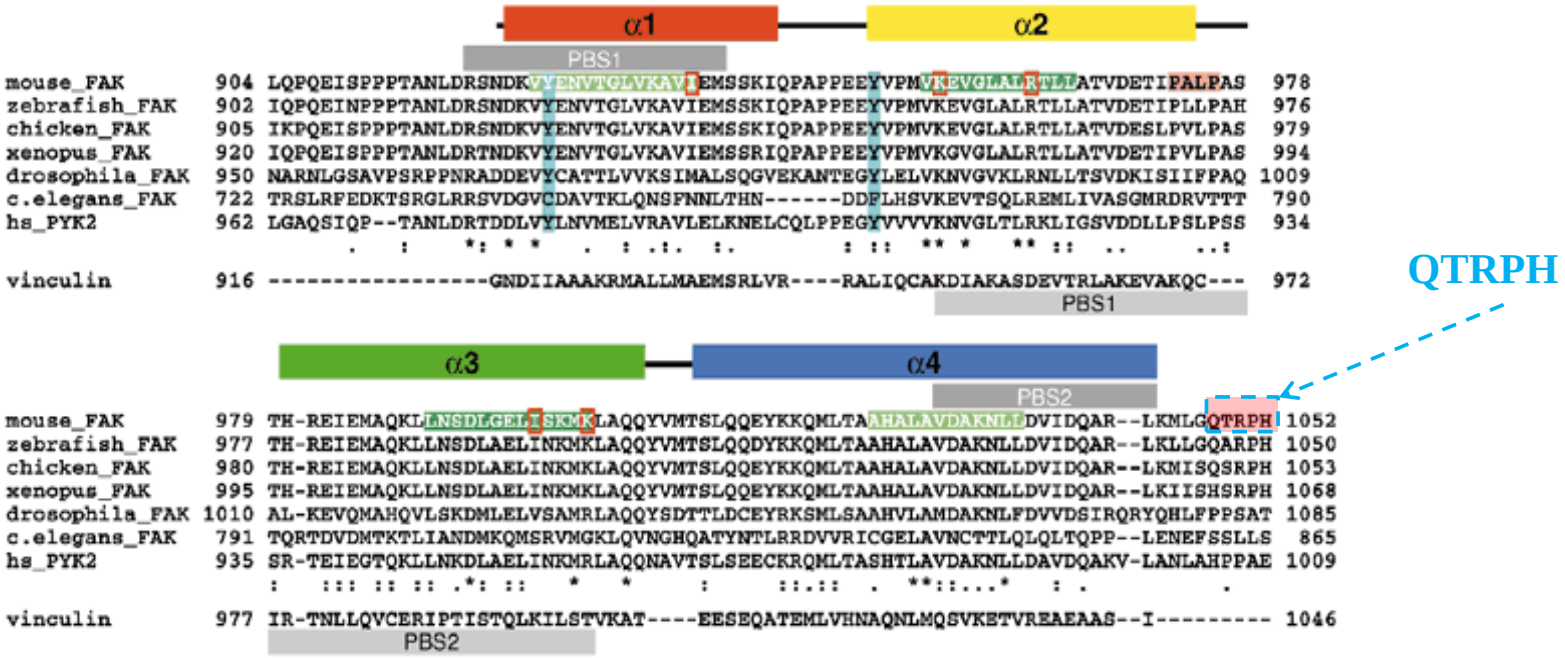


Figure 3-2: FAT sequence for different species. Here, the mouse FAK sequence was used to identify the last five missing residues (QTRPH) of the FAK sequence (modified [13]).

3.1.2.2 LD Motifs Extension-Loop Addition

Since the paxillin connects the FAT domain via LD motifs, it connects to the focal adhesions via the LIM domain, it is reasonable to consider the paxillin as a series of tethers. To provide reactions to the applied force, zero displacements were enforced at the ends of the LD motifs during the simulations. Thus LD motifs produce reaction forces to the force applied to N-terminus of the H1 tail. However, to give the FAT domain more conformational freedom, as would be expected in vivo, five residues were added to either end of the LD4 motif. Based on the paxillin sequence (in chicken) and using Paymol's "builder" feature, five residues were added to each end of the LD4 motif: N-terminal, SASSA; C-terminal, DFKFM. (Figure 3-4.C).

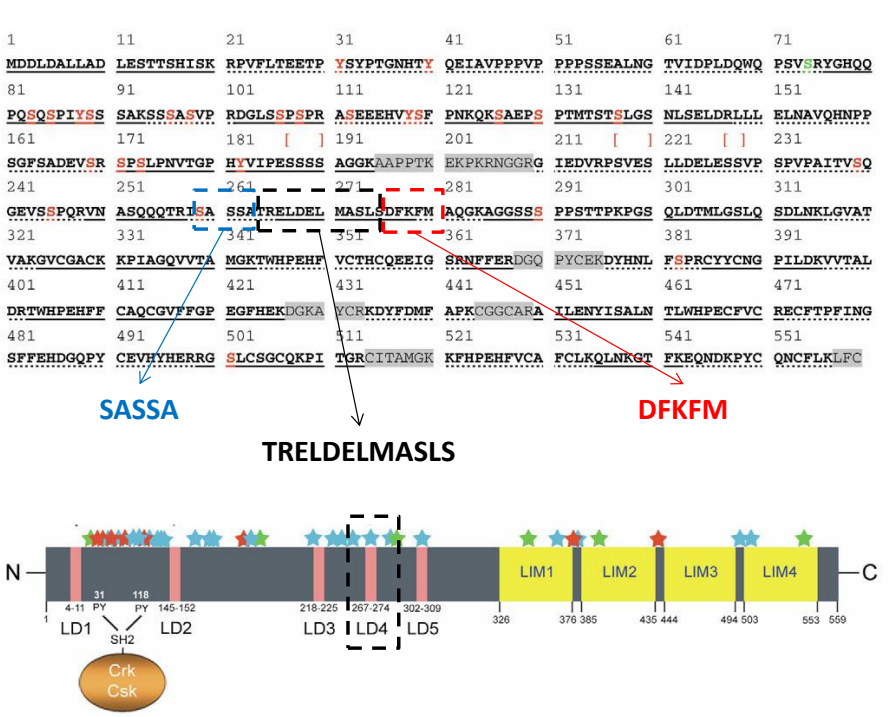


Figure 3-3: Illustration of the paxillin sequence in chicken. The sequence of LD4 is shown in black. The sequence of extensional loop added to the N-terminal of LD4 motif is SASSA (in blue). The sequence of LD4 motif is TRELDELMASLS. The sequence of the extensional loop added to the C-terminal of LD4 motif is DFKFM (modified [28]).

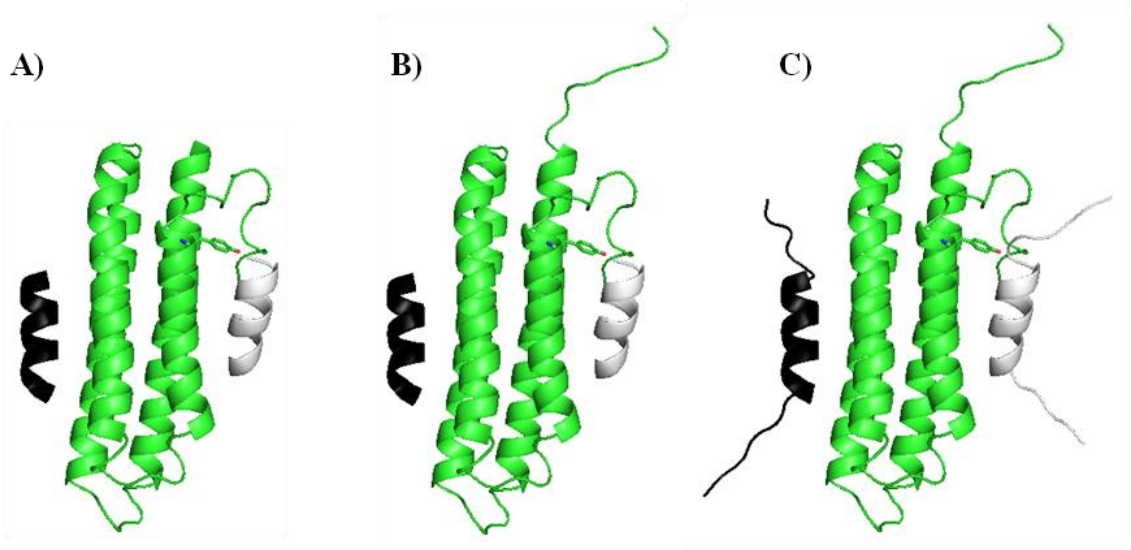


Figure 3-4: Augmented FAT/paxillin complex with H4 tail and P1/P2 constrained. A) The FAT/paxillin complex without H4 tail and P1/P2 unconstrained (constructed from 1ow7.pdb, Figure 3-1. C). B) FAT/paxillin complex after adding missing residues (QTRPH) as a random coil using Pymol for H4 helix. This is referred to as the "H4 tail" throughout. C) FAT/paxillin complex after adding five residues to the LD4 motif (N-terminal, SASSA; C-terminal, DFKFM). This structure was used in the mechanically loaded (AX,PR) with H4 tail (WT) simulations (Table 3-1).

This structure, with the presence and the absence of P2 (LD motif that binds to HP2), was used in all equilibrium simulations (Table 3-1: EQ.WT.P1P2, EQ.WT.P1).

3.1.1 INITIAL STRUCTURES FOR MECHANICALLY LOADED SIMULATIONS

Two load scenarios were chosen (discussed later in §3.2 Simulations) axial (AX) and perpendicular (PR). To examine the role of the mechanical load on H1 behavior, CFMD simulations were performed on as many different mechanical structures as possible. Using the augmented FAT/paxillin structure (Figure 3-4C), the H1behavior in all MD simulations was very similar, but the H1/H4 tail behavior was different. Based on these differences in the tail behavior, different seeds were selected. The term 'seed', which is used later, refers to distinct initial structures, which were selected from MD simulation trajactories at distinct time steps. From the equilibrium simulations (Table 3-1;

EQ.WT.P1P2, EQ.WT.P1), distinct seeds are selected as initial structures for the mechanical loaded CFMD simulations. The criteria for selection is explained as below:

3.1.1.1 H1/H4 Tail Interactions

After the addition of the H4 tail to the structure, possible electrostatic interactions, which may be found between the two tails were examined. These interactions have the potential to influence the load sharing between the H1/H4 tail. Moreover, they may keep H1 attached to the bundle, as well as regulate or otherwise slow down the unfolding events. Figure 3-5 illustrates a representative interaction in which the H1/H4 tail interact via hydrogen bonds. All 390 possible interactions between H1 tail (I909-N921) and H4 tail (L1043-H1052), were screened over all simulations' trajectories. If any distance between two opposite-charged atoms is less than 0.4 nm, it was recorded as an electrostatic interaction. The equation used to calculate the distance between the opposite charges atoms is given in § 3.3.4 Analysis.

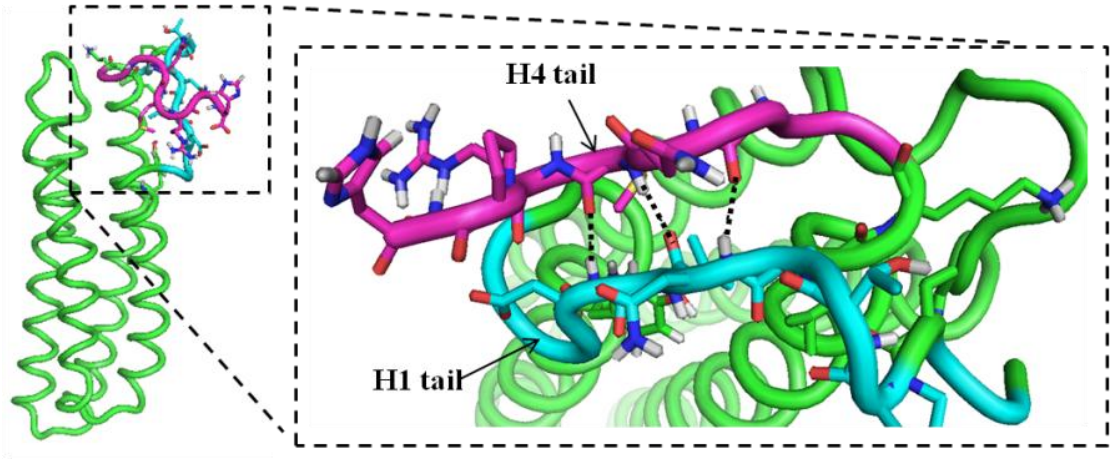


Figure 3-5: Illustration of H1/H4 tail interactions (here are three hydrogen bonds) that were observed during one simulation. The H1 tail is shown in cyan and the H4 tail in magenta.

3.1.1.2 H1/H4 Tail Positions

Based on some preliminary mechanically loaded simulations, it was determined that the relative positions of the H1 and H4 tails could be an appropriate criteria on which to choose the initial structures to be used for the mechanically loaded cases. The metric that developed is a combination of torsion angles that describe the rotation of the tails with respect to a fixed reference. It was necessary to select a stable reference or datum as the entire structure moves. Here, six points, describing the center of mass of each respective turn, were used Figure 3-6. Torsion angles "γ and α" describe the rotation of each tail with respect to each other. However, to make sure that those angles are truly representative, the torsion angle η which measures the twisting angle between H1 and H4, must be stable. The formula used to calculate these angles is the same formula used for ψ calculation (see § 3.3.2.2.1 Analysis).

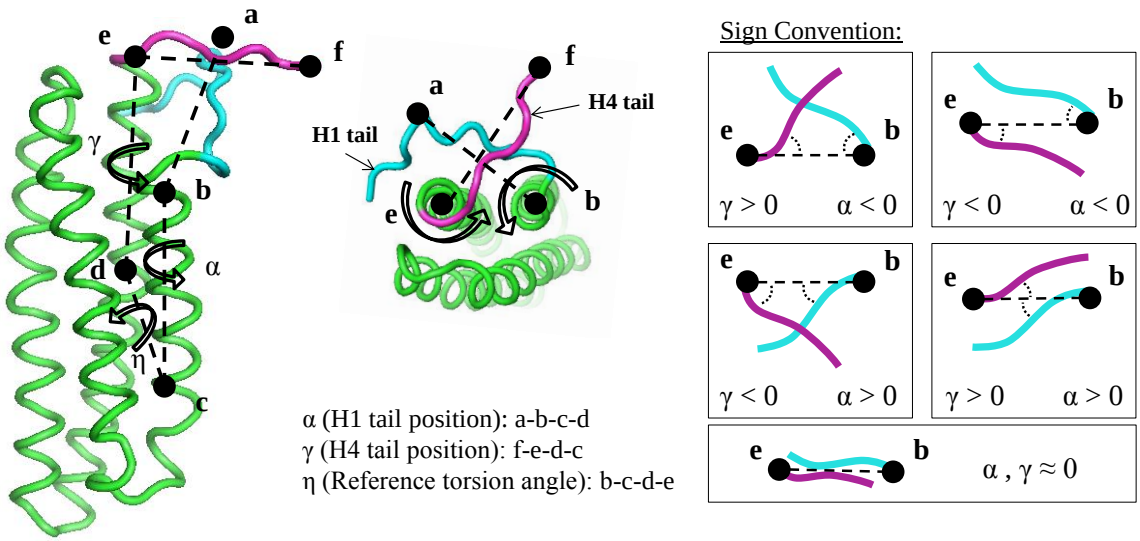


Figure 3-6: Reference system for defining the position of H1/H4 tail with respect to each other. The angle α (a-b-c-d) illustrates the rotation of H1 tail with respect the reference frame formed by (b-c-d-e). The angle γ (f-e-d-c) illustrates the rotation of H4 tail with respect the reference frame formed by (b-c-d-e). The angle η (b-c-d-e) illustrates the twisting of reference frame (H1/H4 axes). The sign of these angles follow the right hand rule where the dash line between the points "e" and "b" is the reference. If α and γ have the same sign, they are separated. However, if they have different sign, they cross each other. When they are equal to zero, it means they are above each other.

3.1.1.3 Selected Seeds for Axial Load Simulation

3.1.1.3.1 H1/H4 Tail Interaction

As seen in Figure 3-7, many interactions developed and/or persisted during the simulations. In some simulations (e.g., Run 4), the tails interacted for nearly 95% of the simulation time, while in others (e.g., Run 2), the tails did not interact at all. In addition to the interaction matrix, the position of the H1/H4 tails with respect to each other is another useful criteria for selecting the appropriate initial structures (i.e., seeds) that were used for the mechanically loaded simulations.

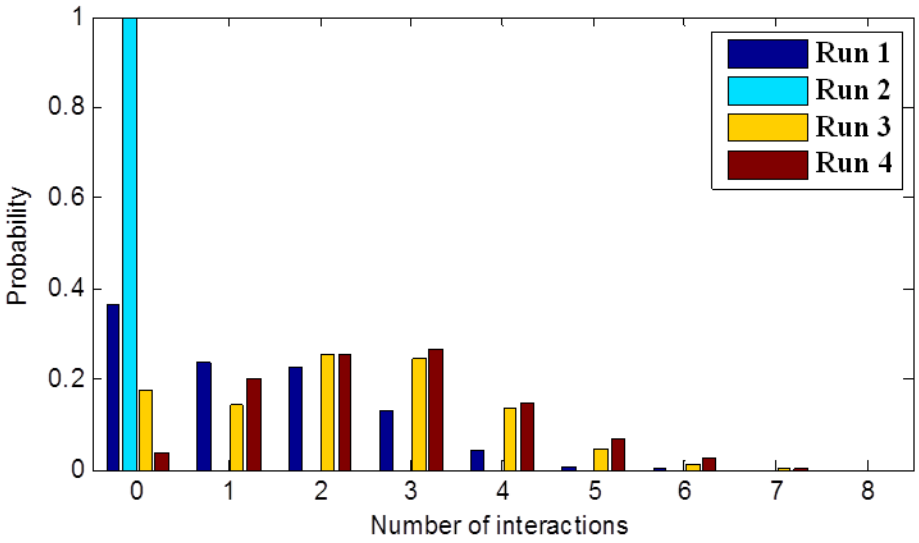


Figure 3-7: H1/H4 tail electrostatic interactions over time. This figure illustrates the different behaviors of the H1/H4 tail. Run #2 is different for each case while all the other runs show a high probability for H1/H4 tail to interact. Seeds were selected to sample these scenarios. Each bar represents a total time 20 ns. (Table 3-1, EQ.WT.P1P2)

3.1.1.3.2 H1/H4 Tail Position

Figure 3-8 shows that (Case ++), η fluctuates $\pm 5^0$ while it stays very close to zero for all different runs. Whether η is a good reference or not depends on how much the tails rotate. The range of the rotation of these tails is about ~ 60^0, so comparing this value with small range of the reference angle suggest that the reference angle that we picked is an acceptable choice. In addition, the figure shows that the position of H1 tail is more stable than the position of H4 that has more mobility. Not only that but also, there is a divergence in the behavior of H4 tail. Run 2 shows that H4 tail does not cross H1 tail, which is supported by the fact that they do not interact most the time (see figure 4-18). All the other runs, however, show a high probability of the H1/H4 tail crossing each other.

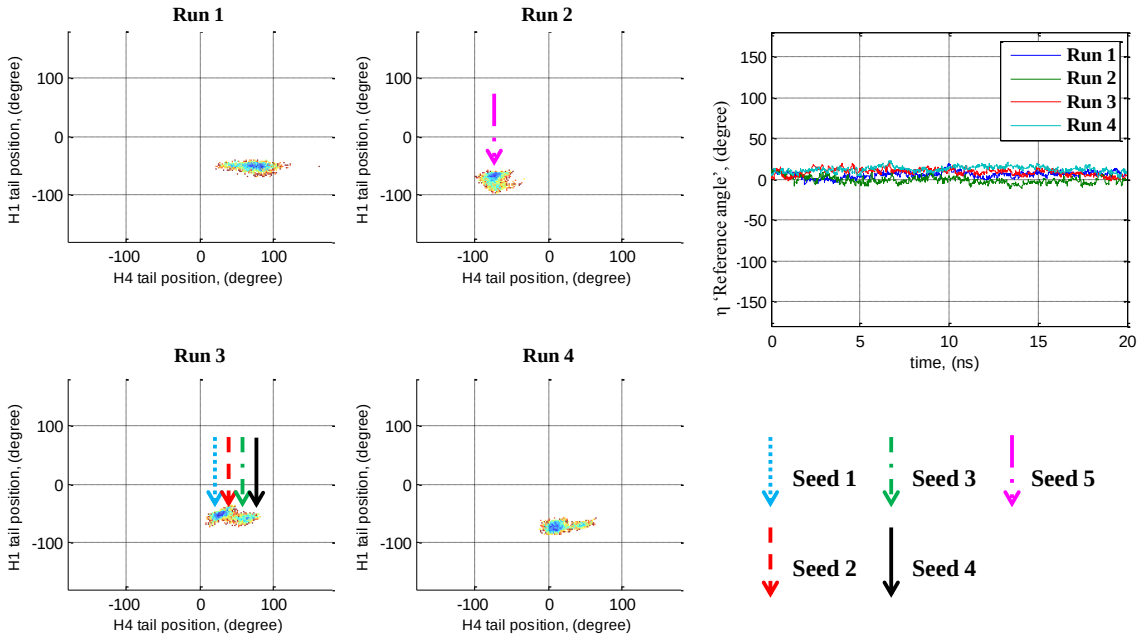


Figure 3-8: Position of H1/H4 tail with respect to each other. This figure shows the different behavior of the H1/H4 tail. The reference angle η is reasonably stable and taken to be a fixed reference. In Run 2, H1/H4 tail is separated while in other simulation they are cross each other. Seeds 1, 2, 3 and 4 were obtained from Run3 while Seed 5 was selected from Run2. (Table 3-1, EQ.WT.P1P2).

3.1.1.3.3 Initial Structures Used for Axial Load Simulations

Figure 3-9 shows a parallel view (parallel to the H1 axis) of the seeds that were selected from the augmented FAT/paxillin simulated under equilibrium. These seeds are the initial structures used in the axial loaded simulation.

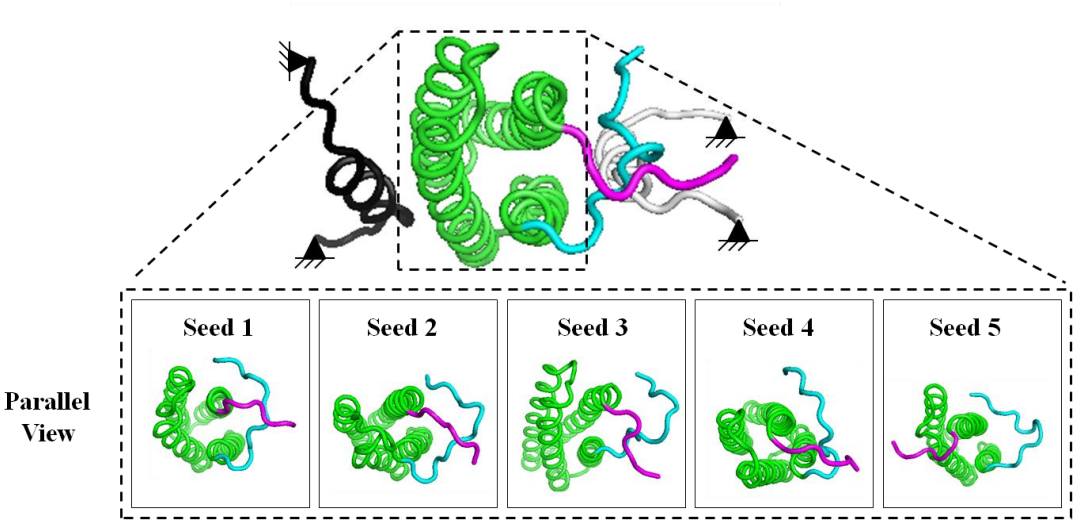


Figure 3-9: Five selected seeds for the axial load simulations (Table 3-1, AX.WT.P1P2). A view from H1's N-terminal in a direction normally parallel to the axis of H1 taken from two different simulation runs (Seed 5 from Run 2, Seeds 1-4 from Run 3) of the equilibrium simulations of augmented FAT/paxillin complex (Table 3-1, EQ.WT.P1P2).

3.1.1.4 Selected Seeds for Perpendicular Load Simulation

3.1.1.4.1 H1/H4 Tail Interactions

As in Figure 3-10, H1/H4 tail electrostatic interactions persisted throughout the majority of the equilibrium simulation (EQ.WT.P1). In three of the four simulations (Run 1, 2 and 4) the tails interacted for approximately 95% of the total time, while in Run 2 the tails interacted little, if at all. In addition to the interaction metric, the relative position of the H1/H4 tail is a useful metric in identifying the possible initial structures (or seeds) to be used for mechanically loaded simulations.

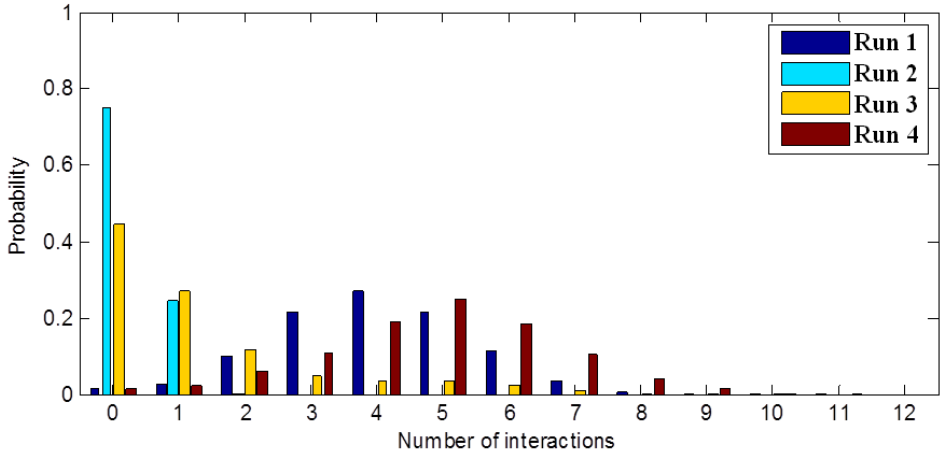


Figure 3-10: H1/H4 tail electrostatic interactions over time. This figure illustrates the diverse behavior of the H1/H4 tail. In Run 2 and Run 3, H1/H4 tail have fewer interactions while in all the other runs they show a high probability for H1/H4 tail to interact. Seeds "initial conditions" were selected to elucidate this wide range of behavior. Each bar represents a total time 20 ns. (Table 3-1, EQ.WT.P1)

3.1.1.4.2 H1/H4 Tail Position

At the absence of P2 to interact with FAT's HP2 (Case +-), Figure 3-11 shows H1/H4 reference angle, η fluctuates $\pm 5^0$ while staying nominally around $\sim 20^0$. The overall range of the rotation of H1/H4 tail is approximately 100^0, so comparing this value with η suggests that the reference used was acceptable. The H1 tail position is more stable than the H4 tail position. Run 2 shows that H4 did not cross H1. Moreover, as seen in Figure 3-10, they do not interact most the time. That said, in three of the four runs the H1/H4 tail show a high proclivity to cross each other.

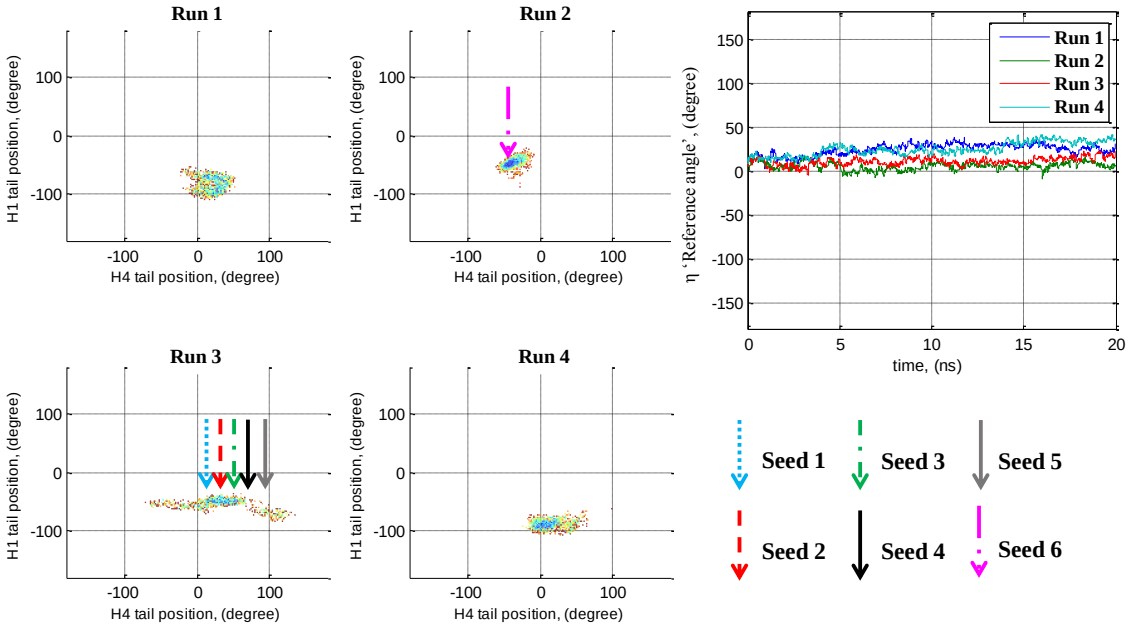


Figure 3-11: Position of H1/H4 tail with respect to each other. This figure shows the different behavior of the H1/H4 tail. The reference angle η is reasonably stable and taken to be a fixed reference. In Run 2, H1/H4 tail is separated while in other simulation they are cross each other. Seeds 1, 2, 3, 4 and 5 were obtained from Run3 while Seed 6 was selected from Run2. (Table 3-1, EQ.WT.P1).

3.1.1.4.3 Initial Structures Used for Perpendicular Load Simulations

Figure 3-12 illustrates the seeds that were selected from augmented FAT/paxillin under equilibrium in the absence of P2 only for the initial structures used in the perpendicular load simulations.

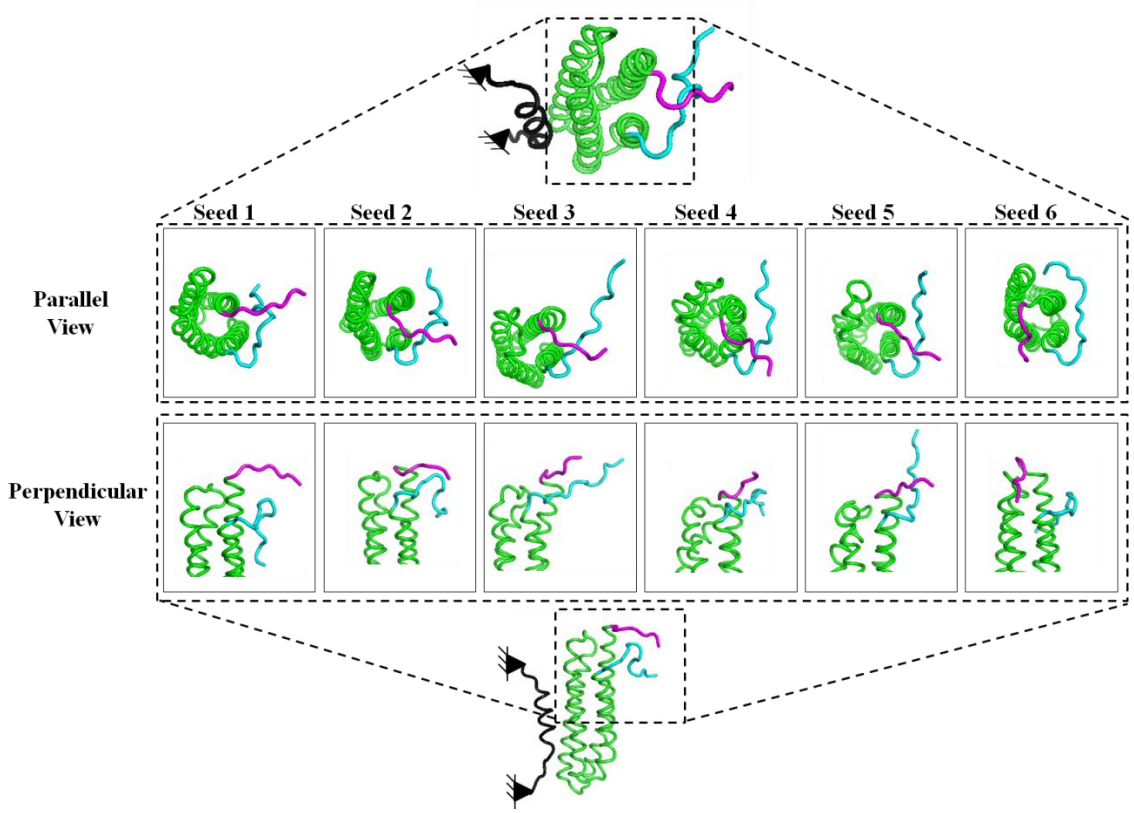


Figure 3-12: Six selected seeds for the perpendicular load simulations (Table 3-1, PR.WT.P1). Views from H1's N-terminal in a direction normally parallel and perpendicular to the axis of H1 taken from two different simulation runs (Seed 6 from Run 2, Seeds 1-5 from Run 3) of the equilibrium simulations of augmented FAT/paxillin complex (Table 3-1, EQ.WT.P1).

3.2 Simulations

A GROMOS53a6 force field was used to run the Molecular Dynamics simulations performed. A time step of 2fs [29] and periodic boundary conditions were implemented for through all phases of the MD simulations. A parallel-processing version of the LINCS constraint on fast-bond dynamics was used [30]. All the simulations were run on Ranger machine at Texas Advanced Computing Center (TACC, www.tacc.utexas.edu).

Different cases of either FAT/paxillin or augmented FAT/paxillin complexes were used in different type of simulations (equilibrium and mechanically loaded simulations). Different cases are defined based on the presence/absence P1 and P2. Each case name is given by [Case +/- +/-]. The first and the second '+/-' indicate the presence/absence of P1 and P2, respectively. For instance, Case + - is interpreted as P1 is present and P2 is absent (Figure 3-13).

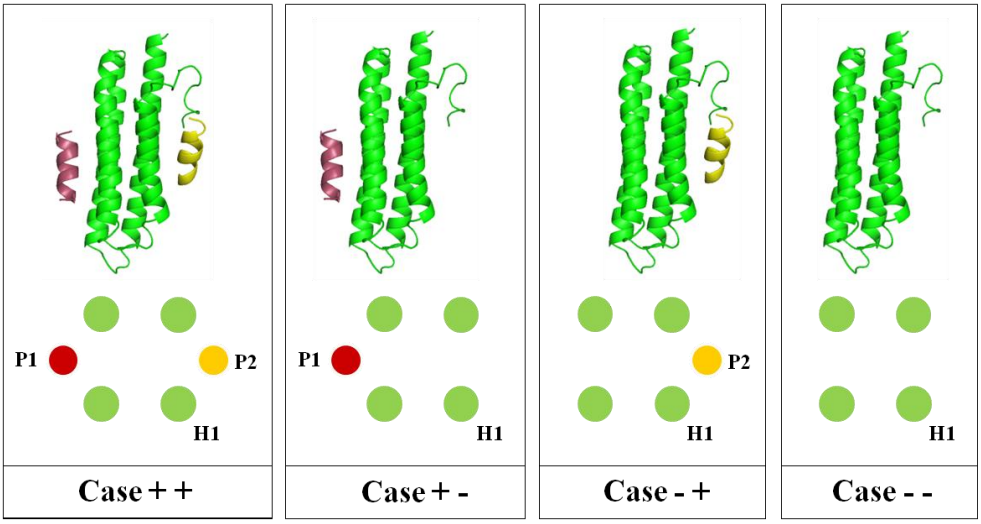


Figure 3-13: Four types of FAT/paxillin without H4 tail used in the equilibrium simulations. The symbol "+" means that the LD motif is present, and "-" means that LD motif is absent from the FAT/paxillin complex. The first + or - indicates the presence or the absence of P1, while the second indicates the presence or the absence of P2.

3.2.1 PRE-EQUILIBRATION

The FAT/paxillin structures were placed in a box of solvent, explicit water (SPC, Figure 3-14). A minimum distance of 1.2 nm in all directions was used for the equilibrium simulation cases, while a minimum distance of 2 nm was used for the loaded simulations In order to neutralize the system's total charge, Na+ and Cl- atoms replaced the solvent atoms (water) at a 0.1 M concentration.

3.2.2 ENERGY MINIMIZATION AND EQUILIBRATION

Following the energy minimization, each structure was heated to 310˚K in three temperature steps (100˚K, 200˚K, 310˚K) with 20 ps spent at each step. The 310˚K structure was then is pressurized to 1 atm within a total time of 750 ps using a Berendsen thermostat [31], a NoseHoover thermostat with a relaxation constant of 0.1 ps [32, 33] to preserve the 310˚K temperature, and a Parrinello-Rahman barostat with a coupling constant of 1 ps [34]. A 1.4 nm cutoff was set for the Coulomb and var der Waals radii. Beyond the cutoff range, the electrostatic interactions were handled using PME electrostatics. By this time, each respective structure had been equilibrated and ready for use in the MD simulations for the equilibrium cases or the CFMD simulations for the loaded cases.

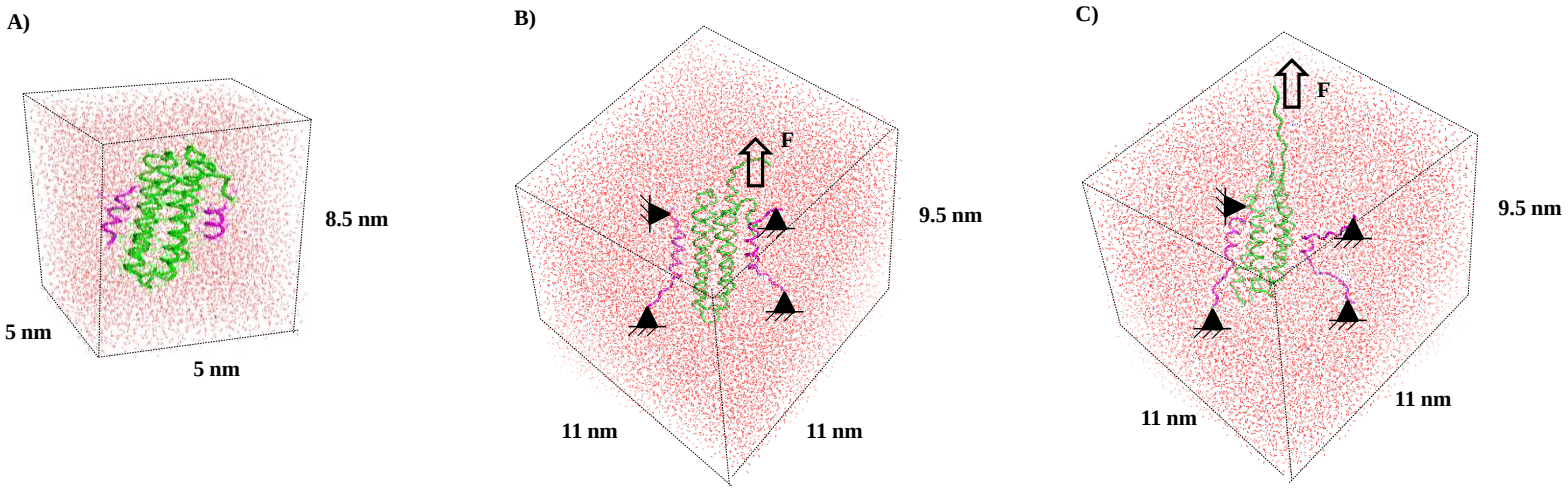


Figure 3-14: MD and CFMD simulation boxes. A) FAT/paxillin complex (1520 protein atoms) in a 5x5x8.5nm rectangular box filled with of explicit water (33,126 SPC water molecules) and 50 counter-ions (25 Na+ and 22 CL-) used for equilibrium simulations (Table 3-1, EQ.WOT.P1P2). B) Augmented FAT/paxillin complex (1821 protein atoms) in a 9.5x11x11nm rectangular box filled with of explicit water (97,719 SPC water molecules) and 125 counter-ions (65 Na+ and 60 CL-) used for axial load simulations (Table 3-1, AX.WT.P1P2), shown at t = 0 ns. C) Augmented FAT/paxillin complex at the end of simulation (t = 20 ns)

3.2.3 EQUILIBRIUM SIMULATIONS

Two different structures were used in the equilibrium simulations: FAT/paxillin complex without H4 tail and P1/P2 unconstrained (Figure 3-1) and augmented FAT/paxillin complex with H4 tail and P1/P2 constrained (Figure 3-4). FAT/paxillin complex without H4 tail and P1/P2 unconstrained was used to study the propensity, if any, for H1 to leave the bundle and/or adopt a β-strand conformation (Table 3-1. EQ.WOT.P1P2, EQ.WOT.P1, EQ.WOT.P2, EQ.WOT.Ø). The four cases are different in terms of the absence and the presence of LD motifs. The augmented FAT/paxillin complex with H4 tail and P1/P2 constrained was used to study the nature of the reported H1/H4 tail interactions and to identify the mechanically loaded simulations..

3.2.3.1 FAT/Paxillin Complex without H4 Tail and P1/P2 Unconstrained

MD simulations were run for four different cases (Figure 3-13) in the presence/absence of P1 and P2. Each of the four cases was run through its own independent energy minimization and equilibration process. Each case had four runs (repeats), each run lasting 20 ns and starting with different initial conditions (Table 3-1). The relative effects of P1 and P2 on H1 behavior are examined.

3.2.3.2 FAT/Paxillin Complex with H4 Tail and P1/P2 Constrained

MD simulations were run for two different cases (Figure 3-4.C) in presence and absence of P2. Each was run through its own independent energy minimization and equilibration process. Each case had four run (repeats), each lasting 20 ns and starting with different initial conditions (Table 3-1, EQ.WT.P1P2, EQ.WT.P1).

3.2.3.3 H1 Isolation

In order to examine what, if anything, keeps H1 folded, MD simulation of H1 (K923-K941) in isolation was run (Table 3-1, EQ.H1). Hydrogen bonds and the hydrophobicity of the bundle influence the conformational structure of H1. A comparison of H1 behavior as it is in isolation and its behavior as it is within the bundle could illustrate what keeps it folded.

3.2.3.4 Paxillin LD Motif Isolation

Based on their crystal structures, the paxillin LD motifs are presumed to be α-helices in nature [12]. To examine this assumption, an LD motif (LD4: T264-S275) was isolated and an MD simulation was run for 40 ns to see its preferred conformational structure (Table 3-1, EQ.LD4).

3.2.4 MECHANICALLY LOADED SIMULATIONS

Load is believed to be applied to the FAT domain through H1's N-terminal where it connects to the rest of the FAK. That said, the direction of the applied load is not known. Two orthogonal load directions were considered in the CFMD simulation: parallel to the H1 axis, or axial; and perpendicular to the H1 axis, or perpendicular.

3.2.4.1 Axial Load Simulations

The first load scenario applied to the augmented FAT/paxillin complex was chosen based on the following:

1. The load presumably must be applied to H1 at its N-terminal where it connects the FAT domain to the rest of FAK. The load is distributed on the atoms of the first residue (I909) of the H1 tail. GROMACS's CFMD loading method divides the total load (100 pN) over all atoms of the loaded group (I909) on a mass weighted basis. The force on atom i is given by $F_i = \left(\frac{m_i}{M}\right) F_{total}$, where m_i is the mass of the atom and M is the sum of the masses.
2. It proved too complicated to apply the load in a transverse direction (perpendicular to H1 axis, normal to the plane containing P1/P2 axes), as shown in Figure 3-15. As it had been tried, an induced steric clash between H1 and P2 is caused by pulling the N-terminus of H1 tail in a direction perpendicular to the plane containing the axes of P1 and P2. However, in order to unravel the area flanking Y925, which is the first portion of H1 to which the load is applied, the load had to be applied axially to H1 axis. GROMACS's CFMD loading method maintains the magnitude and direction of the load constant during the entire simulation.

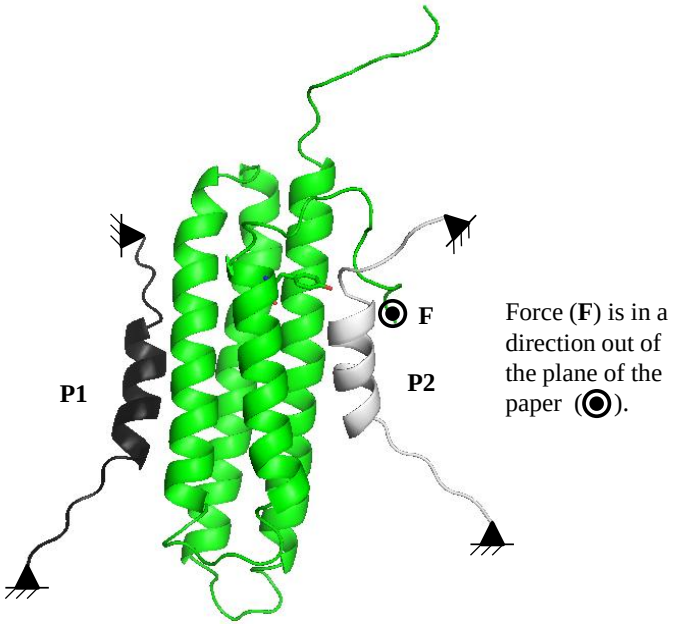


Figure 3-15: Illustration of the induced steric clash between H1 and P2 caused by pulling the N-terminus of H1 tail in a direction perpendicular to the plane containing the axes of P1 and P2 (in the direction out of the plane of the paper).

1. If the load is applied to H1's N-terminal, something else has to provide reaction forces. The FAT domain binds to the paxillin through the LD motifs, where they can be considered tethering reactions, so the ends of P1 and P2 had to be constrained. A zero displacement was enforced at the end of the P1 and P2 specifically, at the Cα atom of S259 (N-terminus of LD4) and Cα atom of M280 (C-terminus of P1). (Figure 3-16.A)

For this load direction, 10 different simulations had different initial structures coming from the MD simulations (Table 3-1, AX.WT.P1P2). The initial structures were selected to be representative of the different equilibrium structure that were observed. The simulations were run using a 100 pN load in a direction parallel to the H1 axis. The reason for such high load was the amount of time a low load simulation may require. So, 100 pN was used to accelerate the process in which H1 comes out of the bundle and/or

adopts β-strand conformation. If this high load achieved the goal in a short time, a simulation would have been performed using a lower load level.

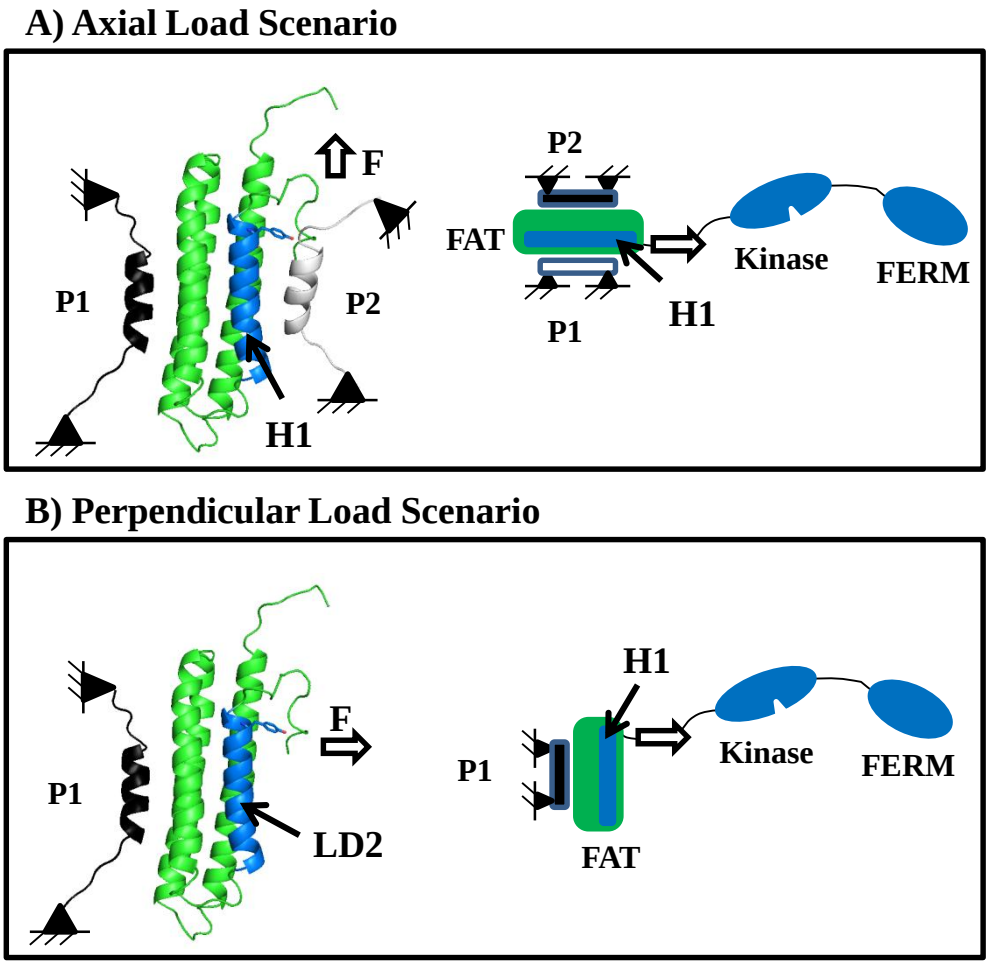


Figure 3-16: Axial and perpendicular loads applied to the augmented FAT/paxillin complex with H4 tail and P1/P2 constrained. A) In the presence of both LD motifs (P1 and P2), the mechanical load is applied to the N-terminus of H1 tail in a direction parallel to the H1 axis. B) In the absence of P2, the load is applied to the N-terminus of H1 tail in a direction perpendicular to the plane containing the H1 and H4 axes.

3.2.4.2 Perpendicular Load Simulation

Review of the literature suggests that access to Y925 is blocked by extensional loops that come from H1 (i.e., H1 tail) and H4 (i.e., H4 tail) in the presence of P2 (i.e.,

LD2). Others have argued that P2 has to be removed first and the tails pulled away from the Y925 site in order for H1 to come out of the bundle. To examine this, P2 was deleted from the augmented FAT/paxillin complex and the load was applied perpendicular to the FAT domain through the H1 tail, and the ends of the P1 motif were constrained (Figure 3-16). A perpendicular load direction was chosen for this case because, after performing several simulations from various directions, the FAT domain self-oriented following the load direction (Figure 3-17). This suggested that the results was insensitive to the load direction. Six seeds were selected (Figure 3-12), the same as described in the axial load scenario.

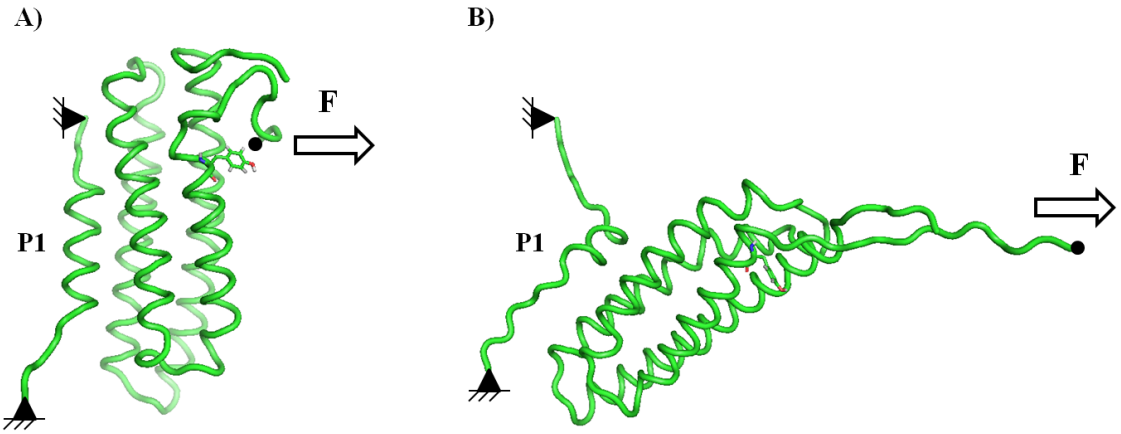


Figure 3-17: Illustration of how the FAT domain self-orients to follow the load direction (PR.WT.P1). A) FAT domain before applying the load to the H1's N-terminus. B) FAT domain after it self-oriented to follow the load direction. It was presumed that all the directions that are perpendicular to the axis of P1 are nearly equivalent.

3.2.5 SIMULATION TIMES

Table 3-1 presents an overall description of the structures, cases and simulation time that were used. Symbol representation was used to illustrate the simulation type and initial conditions of the performed simulations.. The name of each simulation case is defined as [Simulation type. H4 tail status. P1 and P2 status]. The equilibrium simulations was labeled as 'EQ' and the mechanical loaded simulations types were denoted according to their loading direction: 'AX' for axial load scenario and 'PR' for perpendicular load scenario. The presence/absence of H4 tail was labeled by 'WOT' (without H4 tail) and 'WT' (with H4 tail). The presence/absence of P1 and P2 denoted by 'P1', when P1 is in presence; 'P2', when P2 is in presence. If both P1 and P2 are absence, it is labeled by Ø. Each structure had many runs (repeats), where each has different initial conditions. Different energy minimization and equilibration process was labeled by 'EE' and different initial velocities were denoted by 'IV'. In the case where different initial structure (Seeds) were used, it is labeled by 'DS'. The duration time of the run was also identified. Each simulation condition and duration was illustrated as: [Independent initial condition] x [Duration time].

Table 3-1: Equilibruim and mechanically loaded simulations.

Simulation type		Structure	Paxillin		Initial conditions x Time [Independent] x [Duration]	Name
			P1	P2		
Equilibrium (EQ)	w/o H4 tail (WOT)	FAT/paxillin complex (Figure 3-1.C)	+	+	[4 (EE)] x [20 ns]	EQ.WOT.P1P2
			+	-	[4 (EE)] x [20 ns]	EQ.WOT.P1
			-	+	[4 (EE)] x [20 ns]	EQ.WOT.P2
			-	-	[4 (EE)] x [20 ns]	EQ.WOT.Ø
	w/ H4 tail (WT)	Augmented FAT/paxillin complex (Figure 3-4.C)	+	+	[2 (EE) x 2 (IV)] x [20 ns]	EQ.WT.P1P2
			+	-	[2 (EE) x 2 (IV)] x [20 ns]	EQ.WT.P1
	H1 isolated (K923-K941)				[1 (EE)] x [20 ns]	EQ.H1
	LD4 isolated (T264-S275)				[1 (EE)] x [40 ns]	EQ.LD4
	Total time of equilibrium simulations =				**540 ns**	
Mechanically Loaded	Axial (AX)	Augmented FAT/paxillin complex (Figure 3-4.C)	+	+	[5 (DS,EE) x 2 (IV)] x [20 ns]	AX.WT.P1P2
	Perpendicular (PR)		+	-	[5 (DS,EE) x 2 (IV)] x [20 ns] [1 (DS,EE) x 11 (IV)] x [20 ns]	PR.WT.P1
	Total time of mechanically loaded simulations =				**620 ns**	
Total =					**1160 ns**	

Notations:

EE: Different Energy Minimization and Equilibration. IV: Different Initial Velocities.

DS: Different Seeds. +: LD motif is in present. - : LD motif is removed from the structure.

3.3 Analysis

The output data was analyzed using different metrics that addressed different aspects of the availability of Y925 as well as the mechanical behavior of FAT under various load conditions.

3.3.1 Energy Landscape Analysis

In cases where one must look at the stability of the structure and its favorable states, energy landscapes plots would be used. Energy landscapes are evaluated using Boltzmann inversion of the probability of variables *x* and *y* occurring at time t as follows:

$$\boldsymbol{E(x,y) = -\ln\,[P(x,y)]}$$

where *p(x,y)* is the probability of the variables *x* and *y* over time.

The blue color (minima) represents a point/region of the highest likelihood. According to this scaling, an point lying in the blue region is about 500 times more likely than an equivalent point lying in the red region (Figure 3-18).

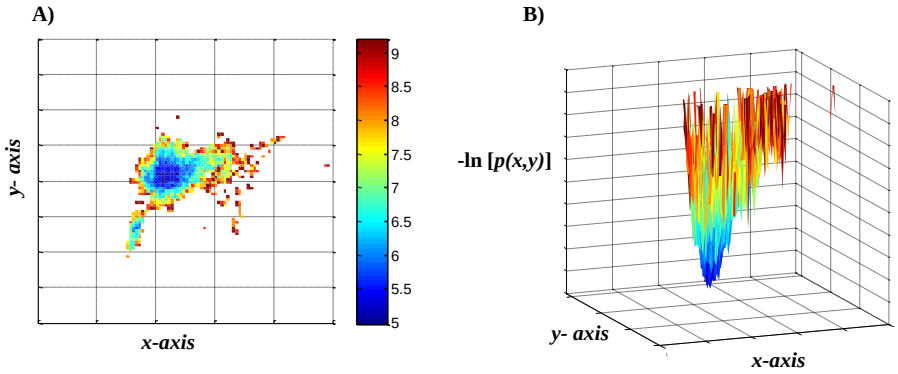


Figure 3-18: Illustration of energy landscape where the colors represent the depth of the well. A) Top view. B) Third dimension which is the depth of the well.

3.3.2 H1 BEHAVIOR

The main interest is to examine the behavior of H1 in terms of its position and its helical character. Distance metric was chosen to track the position of H1 relative to the bundle. Backbone dihedral angle ψ is calculated for the first five residues (K923, V924, Y925, E926, and N927) of the N-terminal of H1.

3.3.2.1 H1 Position

To examine the hypothesis that H1 must be out of the bundle in order to allow Y925 phosphorylation, H1's position was evaluated. The position of H1 relative to the bundle is taken to be the distance between H1 and the helices adjacent to it, H2 and H4. To have single plot that is able to indicate the position of the entire H1 (top and bottom portions), the distance between H1 and an virtual helix, which is the equivalent between H2 and H4, was calculated. The energy landscape of top distance d_{top} vs. the bottom distance d_{bottom} was plotted to determine the most likely position of H1 (Figure 3-19.A).

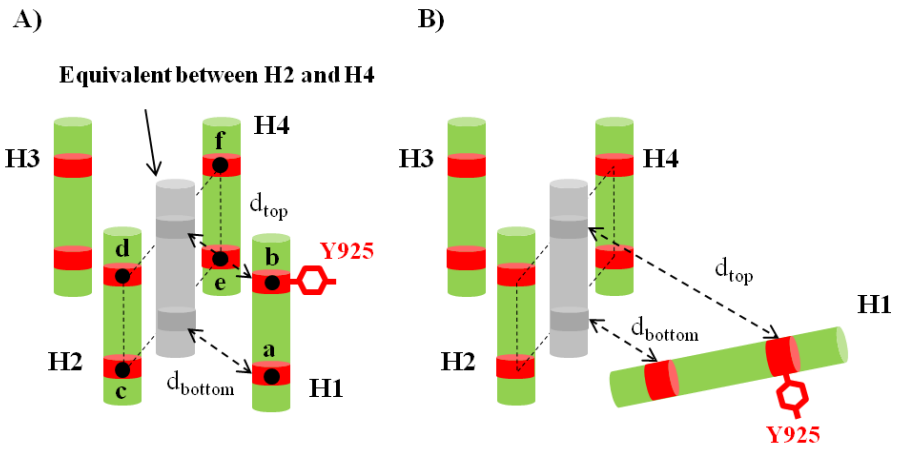


Figure 3-19: H1 position characterization. A) Top and bottom distances between H1 and a virtual helix (in gray). The top distance is between the N-terminal of H1 (center of mass of K923-N927) and the average point of the C-terminal of H2 (center of mass of T963-T967) and N-terminal of H4 (center of mass of L1035-D1039). The bottom distance is between the C-terminal of H1 (center of mass of E937-K941) and the average point of the N-terminal of H2 (center of mass of V951-K955)

and C-terminal of H4 (center of mass of T1022-A1026). B) The potenital position of H1 if it leaves the bundle.

The top distance and bottom distance, which were used in the analysis, are calculated as follows:

$$d_{top} = \sqrt{\left[b_x - \frac{d_x+f_x}{2}\right]^2 + \left[b_y - \frac{d_y+f_y}{2}\right]^2 + \left[b_z - \frac{d_z+f_z}{2}\right]^2}$$

$$d_{bottom} = \sqrt{\left[a_x - \frac{c_x+e_x}{2}\right]^2 + \left[a_y - \frac{c_y+e_y}{2}\right]^2 + \left[a_z - \frac{c_z+e_z}{2}\right]^2}$$

Where points 'a and b' are the centers of mass of two complete turns at the C- and N-terminals of H1 respectively (a: E937-K941, b: K923-N927). Points 'c and d' are the centers of mass of complete turns at the N- and C-terminals of H2 respectively (c: V951-K955, d: T963-T967). Points 'e and f' are the centers of mass of complete turns at the N- and C-terminals of H4 respectively (e: T1022-A1026, f: L1035-D1039) (Figure 3-19). Since the C-terminal of H1 connects with H2 and the N-terminal of H1 is pulled out, one expects it to be more likely that the top distance of H1 will increase as H1 opens out (Figure 3-19.B).

3.3.2.2 H1 Unfolding

According to the known Ramachandran (φ,ψ) plot, for H1 to adopt β-strand conformation, itsbackbone dihedral angle has to be ~ 170^0. For more detailed to understand the unfolding propagation, if any, the instantaneous status of hydrogen donor-acceptor pairs metric is examined.

3.3.2.2.1 Backbone Dihedral Angle ψ

A current hypothesis suggests that the region flanking Y925, "N-terminal of H1," has to adopt β-strand conformation [5]. This can be tested using the backbone dihedral ψ (N_i-$C\alpha_i$-C_i-N_i) which demonstrates the conformation of the backbone main chain. For an

α-helix, ψ ≈ -50^0, while for a β-strand: ψ ≈ 170^0 (Figure 3-20). Using for points (N_i,$C\alpha_i$,C_i,N_{i+1}), ψ that were evaluated in the analysis is calculated as follow:

$$\psi = \text{atan2}(|\mathbf{b}_2|\mathbf{b}_1 \,.\, [\mathbf{b}_2 \times \mathbf{b}_3], [\mathbf{b}_1 \times \mathbf{b}_2] \,.\, [\mathbf{b}_2 \times \mathbf{b}_3])$$

where $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$ are vectors defined as: $\mathbf{b}_1 = \overline{C\alpha_i - N_i}$, $\mathbf{b}_2 = \overline{C_i - C\alpha_i}$, and $\mathbf{b}_3 = \overline{N_{i+1} - C_i}$.

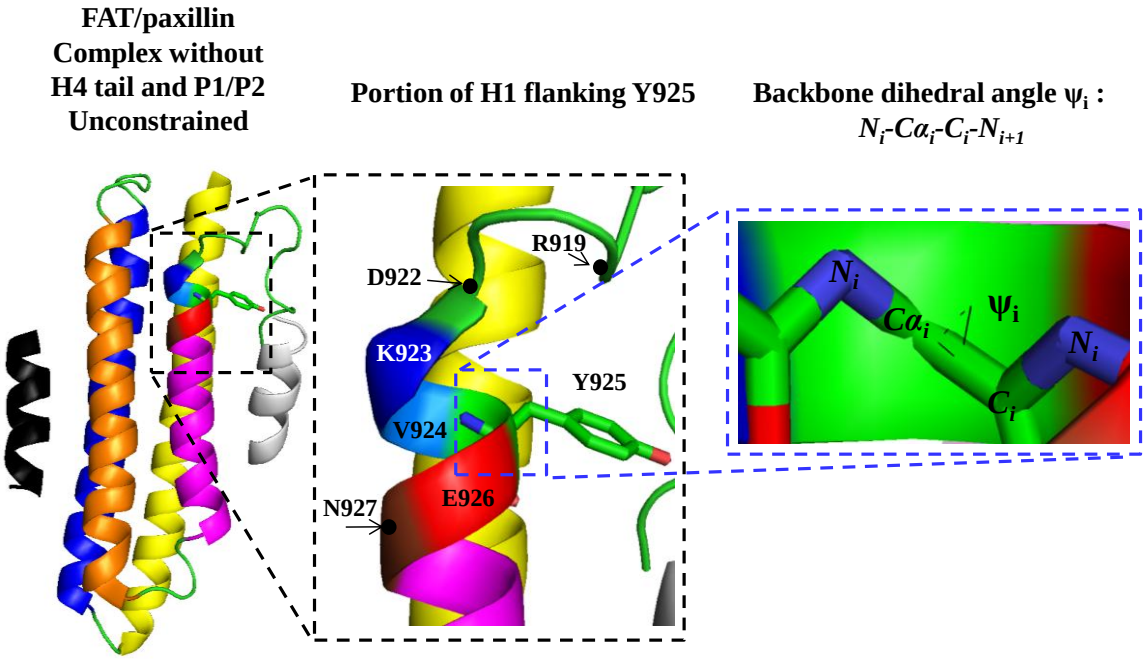


Figure 3-20: Residues neighboring the Y925 residue. An expanded view of the region flanking Y925 at the N-terminal of H1. The backbone dihedral angle ψi (N_i-$C\alpha_i$-C_i-N_{i+1}) that describes H1 secondary structural conformation. For an α-helix, ψ ≈ -50^0 and for a β-strand, ψ ≈ 170^0.

3.3.2.2.2 Hydrogen Bonds via Donor-Accepter Pairs

Details regarding unfolding are revealed via the states of the hydrogen donor-acceptor pairs (Figure 3-21). To maintain the helical character in a secondary structure level of the protein, hydrogen bonds are formed between a backbone oxygen from one residue and an amine hydrogen from another residue. To form a hydrogen bond, two

conditions need to be satisfied: i) The distance between the oxygen (acceptor) and nitrogen (donor) 'd_{HB}' must to be less than 0.35 nm and the angle 'Θ_{HB}' must be less than 30˚.

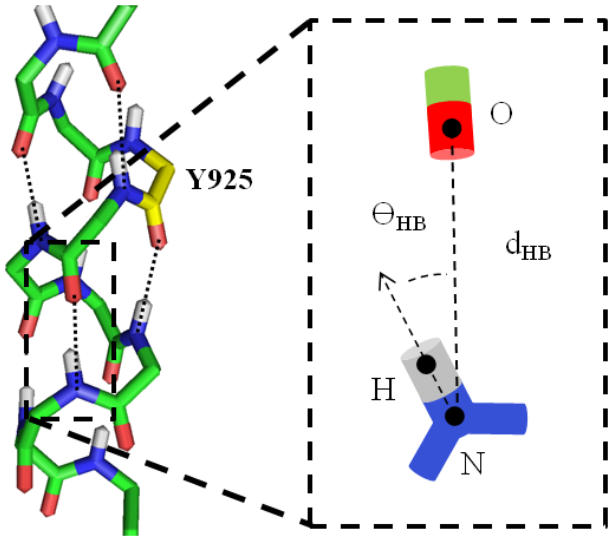


Figure 3-21: Illustration of a hydrogen donor-accepter pair formed as O-N-H (donor N+, accepter O-). A hydrogen bond saw assured to be formed if the distance between O and N (d_{HB}) was to be less that 0.35 nm and the angle Θ_{HB} formed by O-N-H was less than 30^0.

The hydrogen donor-acceptor pair was calculated as follows:

$$\bar{d}_{HB} = [O_x - N_x]\boldsymbol{i} + [O_y - N_y]\boldsymbol{j} + [O_z - N_z]\boldsymbol{k}$$

$$\overline{HN} = [H_x - N_x]\boldsymbol{i} + [H_y - N_y]\boldsymbol{j} + [H_z - N_z]\boldsymbol{k}$$

where *O*, *N*, and *H* are the centers of mass of the atoms forming the hydrogen bonds: oxygen, nitrogen, and hydrogen, respectively, and ***i***, ***j***, and ***k*** are the unit vectors.

The hydrogen bond distance 'd_{HB}' is:

$$d_{HB} = |\bar{d}_{HB}|$$

The hydrogen bond angle 'Θ_{HB}' is:

$$\theta_{HB} = ACOS\left[\frac{\bar{d}_{HB} \cdot \overline{HN}}{|\bar{d}_{HB}| . |\overline{HN}|}\right]$$

Hydrogen acceptor-donor pair analysis provides information about the type of helix: 3_{10}-helix, 'i:i+3'; α-helix, 'i:i+4'; π-helix, 'i:i+5' where 'i' represents the residue number (Figure 3-22).

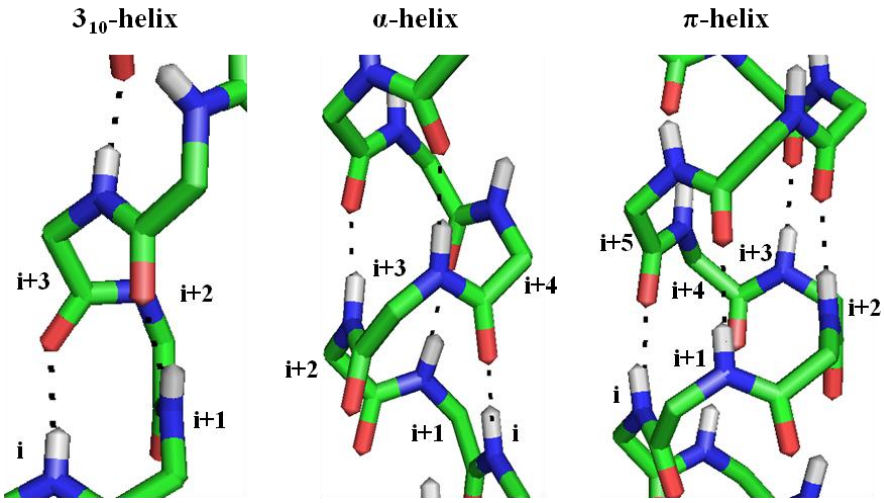
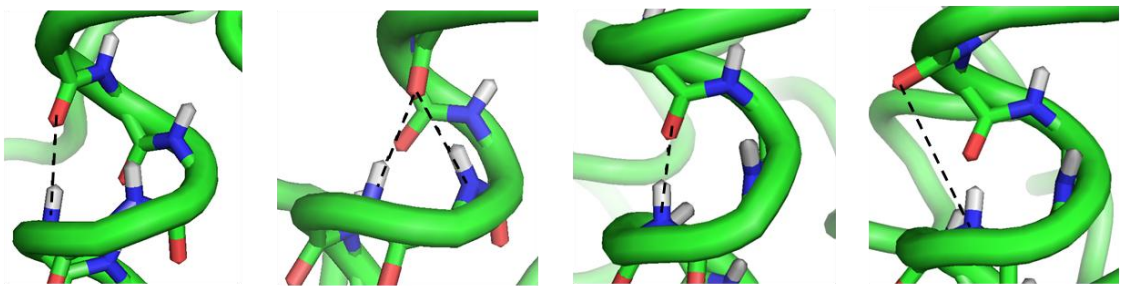


Figure 3-22: 3_{10}, α and π helices formed by various hydrogen donor-accepter pairs starting with residue i.

During all MD and CFMD simulations, only four types of hydrogen donor-acceptor pair appeared. Primarily, the helix formed a hydrogen bond between i:i+4 residues, which is called an α helix-type bond. There is a very low propensity to form the 3_{10} hydrogen bond between i:i+3 residues. In yet another type of hydrogen bond, a combination of α and 3_{10}, the residue "i" forms a double hydrogen bond, $\alpha/3_{10}$, between residues i:i+3/i+4. In addition to these types, no or a broken hydrogen bond that occurs sometimes was labeled "Ø." Figure 3-23 illustrates the types of hydrogen donor-acceptor pairs observed during the simulations.



α $\quad$ α/3_{10} $\quad$ 3_{10} $\quad$ Ø

Figure 3-23: Illustration of the three types of hydrogen donor-acceptor pairs (α, α/3_{10} and 3_{10}) that formed during the simulations, as well as the no hydrogen bond case, denoted by the symbol "Ø."

3.3.3 SALT BRIDGES BETWEEN H1 TAIL AND H4

Based on the published crystal structures, the two important salt bridges between H1 and H4 were observed. Salt bridge 1 (SB1) is formed by the interactions between the side chains of R919-D1039 while Salt bridge 2 (SB2) is formed by the interactions between the side chains of D922-R1042 [5]. The distance between the centers of mass of the terminal, side-chain carbon atoms, CZ and CG, from arginine (R) and aspartic acid (D), respectively, was evaluated (Figure 2-4) as follows:

$$SB_i = \sqrt{[CZ_x - CG_x]^2 + \left[CZ_y - CG_y\right]^2 + [CZ_z - CG_z]^2}$$

where *i*=1,2 represents the first or the second salt bridge.

3.3.4 H1/H4 TAIL INTERACTION

Based on primarily simulation, it appeared that the H1/H4 tail may share the applied load resulting H1 holding to the bundle as well as slowing down any unfolding events. As a result, all possible interactions that can be formed between H1/H4 tail have been surveyed as discussed previously. Examining the correlations between forming such an electrostatic interaction and the unfolding events gives better idea about the influence,

if any, of H1/H4 tail interactions on H1 behavior. The electrostatic interaction distance (d_{EI}) between any opposite charged atoms was calculated as follows:

$$d_{EI} = \sqrt{[(-ve)_x - (+ve)_x]^2 + \left[(-ve)_y - (+ve)_y\right]^2 + [(-ve)_z - (+ve)_z]^2}$$

where '*-ve*' represents the negative charge atom and '*+ve*' represents the positive charge atom. The negative charges atoms are either the backbone oxygen atoms or the terminal side-chain oxygen atoms. The same for the positive charged atoms, they are either backbone nitrogen atoms or terminal side-chain nitrogen atoms.

3.3.5 FINAL STATE OF FAT'S STRUCTURE UNDER APPLIED LOAD

For different CFMD simulations, FAT domain undergoes different structural states. Table 3-2 and Figure 3-24 illustrate a classification of different final states of the FAT structure. The classification is based on H1 position, H1unfolding H1/H4 tail interaction, and the area between the H2-H3 helices. Symbol representation was used to describe these final states. For H1 position, H1 is either in or out of the bundle labeled by 'In and Out' respectively. For H1 Unfolding, there is a degree of unfolding of the first five residues (K923, V924, Y925, E926, and N927), 'H' means they are folded in a helical form and 'SUF' illustrates the unfolding of the first two residues (K923, V924) while 'UF' means that all the five residues unfolded. For H1/H4 tail interactions, when the C-terminal of H4 tail forms a β-sheet with N-terminal of H1 tail via hydrogen bonds, it is labeled by 'β, EX' where the label 'β, NEX' means that the β-sheet is formed between the C-terminal of H4 tail and mid section of H1 tail. In the case where the C-terminal of H4 tail entangled with the C-terminal of H1 tail, it is denoted by 'τ'. If H1/H4 are separate, it is labeled by 'S'. In addition, it was observed that the C-terminal of H2

and the N-terminal of H3 was sometime unfolded, which is denoted by ‘U23’, but if they are folded it is denoted by ‘F23’.

Table 3-2: Classification of different FAT structures in the final states that were observed during the simulations. Each symbol describes a different structure a portion of the FAT domain would adopt. Those states are illustrated in Figure 3-24 .

Classification	Symbol	Qualitative Description
H1 Position	In	H1 stays in the bundle.
	Out	H1 is out of the bundle.
H1 Unfolding	H	H1 is in a helical form.
	SUF	The first two residues of N-terminal of H1 (K923 and V924) start to unfold.
	UF	The region flanks Y925 is unfolded (K923, V924, Y925, E926, and N927)
H1/H4 Tail Interactions	β, EX	H1/H4 tail form β-sheet via hydrogen bonds. The C-terminal of H4 tail interacts with N-terminal of H1 tail.
	β, NEX	H1/H4 tail form β-sheet via hydrogen bonds. The C-terminal of H4 tail interacts with mid section of H1 tail.
	τ	H1/H4 tail have interactions where the C-terminal of H4 tail interacts with the C-terminal of the H1 tail (i.e., near the N-terminal of H1 helix).
	S	H1/H4 tail do not have interactions (i.e., they are separate).
H2-H3 Structure	U23	The C-terminal of H2 and the N-terminal of H3 are unfolded.
	F23	The C-terminal of H2 and the N-terminal of H3 are folded.

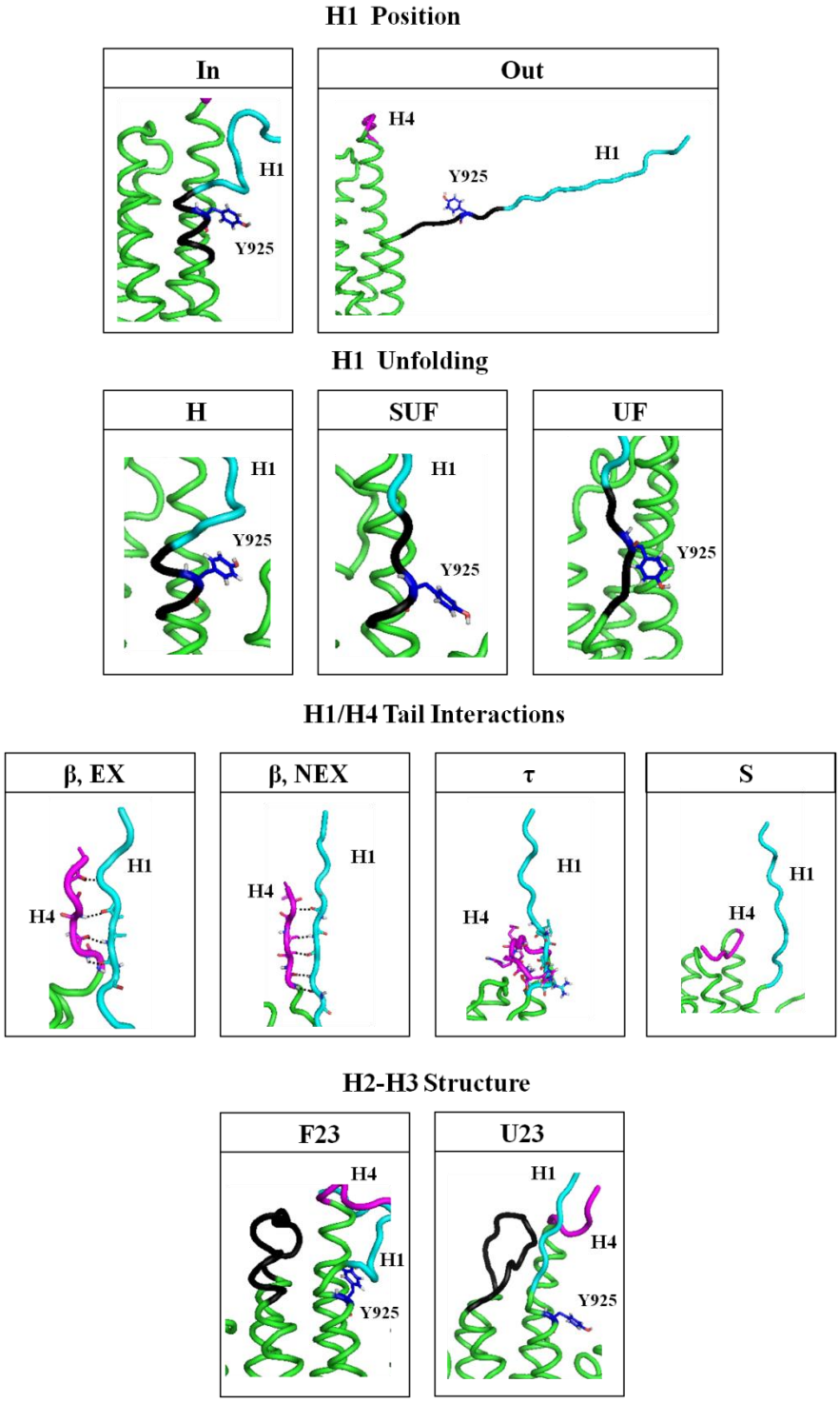


Figure 3-24: Illustrations of different parts of the FAT domain in different final states. Those notations that are described in Table 3-2 used for classification of the final states that FAT domain.

In the next chapter, the results of the metrics chosen are presented and discussed statistically. In addition, the biological implications behind those statistics will be discussed.

Chapter 4. Results

The primary goal is to determine the conditions required for the FAT domain (specifically; its H1 helix) to undergo the hypothesized structural changes, in which H1 comes out of the bundle and/or adopts β-strand conformation. These conformational changes presumably allow Y925 to be phosphorylated. In addition, it is important to examine the influence of the paxillin LD motifs, which bind to FAT, on the behavior of the H1. Under equilibrium and mechanical load, four metrics were evaluated for examining H1 behavior:

1. H1 position
2. H1 unfolding
3. H1/H4 salt bridges
4. H1/H4 tail interactions.

4.1 Equilibrium Results

4.1.1 FAT/PAXILLIN COMPLEX WITHOUT H4 TAIL AND P1/P2 UNCONSTRAINED

Under equilibrium, the FAT/paxillin complex had been investigated in which the presence or absence of P1 and P2 was varied. (Figure 3-4 and Table 3-1, EQ.WOT.P1P2, EQ.WOT.P1, EQ.WOT.P2, and EQ.WOT.Ø).

4.1.1.1 H1 Position

Under equilibrium conditions, the position of H1 does not vary significantly. As seen in Figure 4-1, the blue colored regions (minima) of the H1 position have small distribution. The relative position of H1 to the bundle is very stable, which means H1 does not appear to have a propensity to leave the bundle for any case that was simulated.

Based on the literature, electrostatic and hydrophobic interactions between H1 (residues 917-922) and H4 present an energy barrier keeping H1 attached to the bundle. This observation and H1 position results are consistent. However, in order for Y925 to engage the physphorylation, H1 has to leave the bundle. Therefore, under only thermal fluctuation, it does not seem that H1 has the capacity to leave the bundle. Furthermore, even in the absence of both P1 and P2 (Case - -), the relative position of H1 to the bundle is stable, which means H1 is strongly attached to the bundle regardless of the presence or absence of the paxillin LD motifs. It appears that P1/P2 do not have an significant influence on the stability of H1.

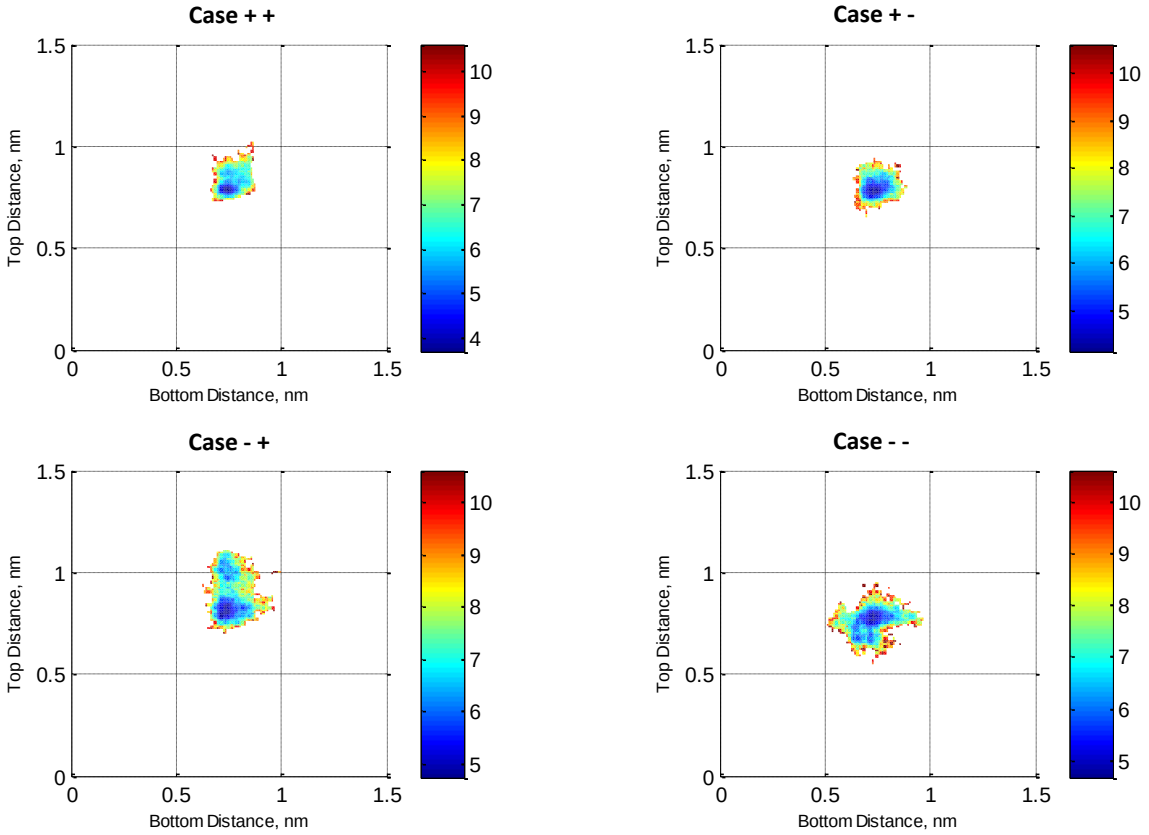


Figure 4-1: Energy landscape of H1 position represented by d_{top} and d_{bottom} in the presence and/or the absence of P1 and P2. H1 position has a small distribution (minima) which means H1 does not appear to have the propensity to leave the bundle under only thermal fluctuation. Each plot represents a cumulative time of 80 ns of simulation time. (Table 3-1, EQ.WOT.P1P2, EQ.WOT. P1, EQ.WOT.P2, and EQ.WOT.Ø).

The Case -+ (P1 is absent), is slightly different than other cases. In all four runs, the H1 position is very similar to those in the other cases seen in Figure 4-1 except the fourth run, which has two local minims (two states, Figure 4-2). However, the top distance of H1 increased by 0.2 nm and stayed stable, which is an indication of the stability of the relative position of H1 with respect to the bundle.

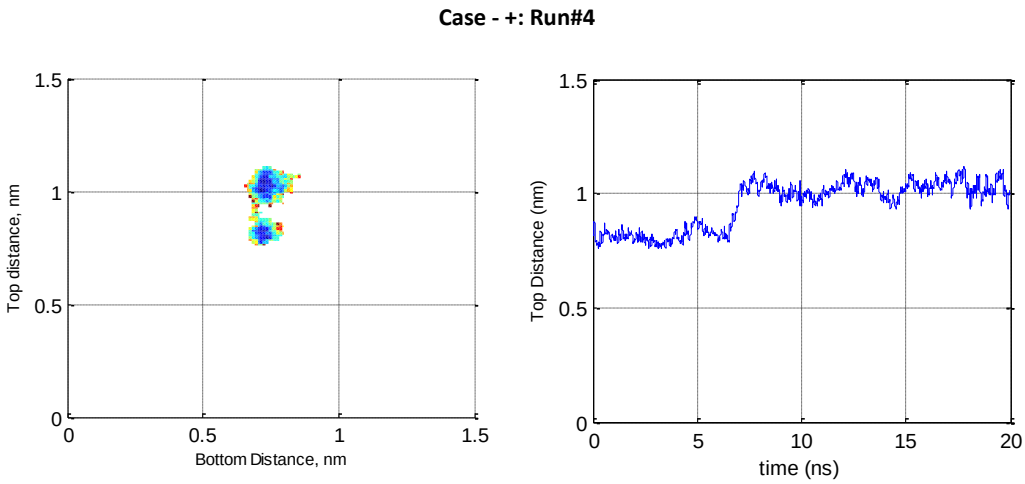


Figure 4-2: Energy landscape of H1 position represented by d_{top} and d_{bottom} in the absence of P1. d_{top} versus time illustrates the presence of the two local minima (blue spots) on the energy landscape plot for Run#4. d_{top} does not fluctuate between two states, which demonstrates the stability of H1 position relative to the bundle. (Table 3-1, EQ.WOT.P2).

4.1.1.2 H1 Unfolding

To examine the unfolding of H1, if any, two important metrics were evaluated: backbone dihedral angle ψ and hydrogen donor-accepter pairs (illustrated previously in § 3.3.2.2 analysis).

4.1.1.2.1 Backbone Dihedral Angle ψ

As in Figure 4-3, except residue K923, the ψ angles of the other top four residues of the N-terminal of H1 (V924, Y925, E926, and N927) have a small distribution (the mean value is ~ -50^0 degree). This means they are folded in a helical form for any case simulated. However, the first residue at the N-terminus of H1 (K923) is expected to have high flexibility, since it connects with H1 tail (i.e., H1 tail is free to move). That said, the flexibility of K923 does not affect the stability of the other residues flanking Y925.

For Y925 to engage the phosphorylation, the region flanking Y925 has to adopt β-strand conformation as it was discussed in §2.5 Literature Review. Under only thermal fluctuation, the ψ metric suggests that residues flanking Y925 do not appear to have propensity to adopt β-strand conformation. In addition, even in the absence of both P1 and P2 (Case - -), H1 has the ability to stay folded in a helical form. This suggests that maintaining the helical form of H1 is nearly independent of the FAT association with paxillin.

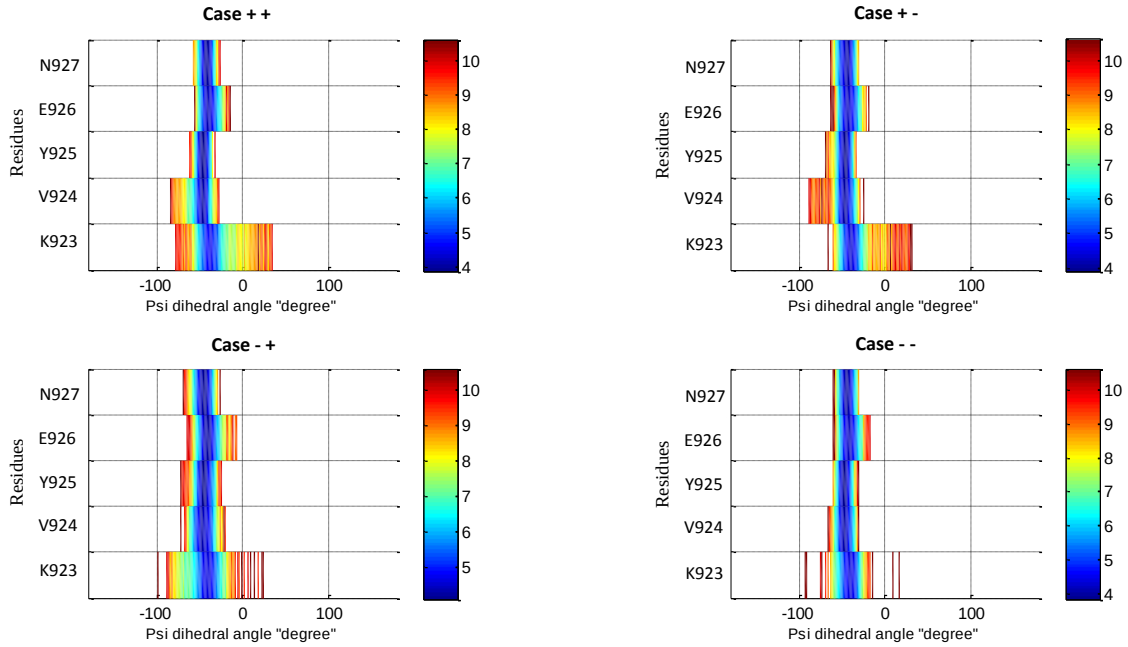


Figure 4-3: Energy landscape of the dihedral angle ψ of the five N-terminal residues of H1 (K923, V924, Y925, E926 and N927) in the presence and/or the absence of P1 and P2. Except N923 that have greater flexibility, since it connects with the floppy tail (H1 tail), ψ angle of other residues has a small distribution (minima). This means H1 does not appear to have the propensity to adopt β-strand conformation under only thermal fluctuation. Each plot represents a cumulative simulation time of 80 ns. (Table 3-1, EQ.WOT.P1P2, EQ.WOT. P1, EQ.WOT.P2, and EQ.WOT.Ø)

4.1.1.2.1 Hydrogen Donor-Accepter Pairs

Figure 4-4 shows the probability of forming different types of hydrogen bond for the first five residues at the N-terminal of H1 (K923, V924, Y925, E926, and N927). Most the time, they form an α-helix hydrogen bond type. On the other hand, π and 3_{10}-helix hydrogen bond type formed very rarely. The hydrogen bond of K923 is broken about ~ 25% of the time. However, the hydrogen bonds of other four residues are broken about 3% to 7% of the time. The residue K923 is expected to have more broken hydrogen bond since it connects to the H1 tail. Hydrogen donor-acceptor pairs metric is useful in examining the propagation of the unfolding, if any. Based on what Figure 4-4 shows, the unfolding of K923 does not propagate into the other four residues where they are stable. Moreover, the absence of both P1 and P2 does not affect H1 behavior in terms of maintaining their α-helical form. This is consistent with the previous suggestion that the stability of the H1 is independent of FAT association with the paxillin.

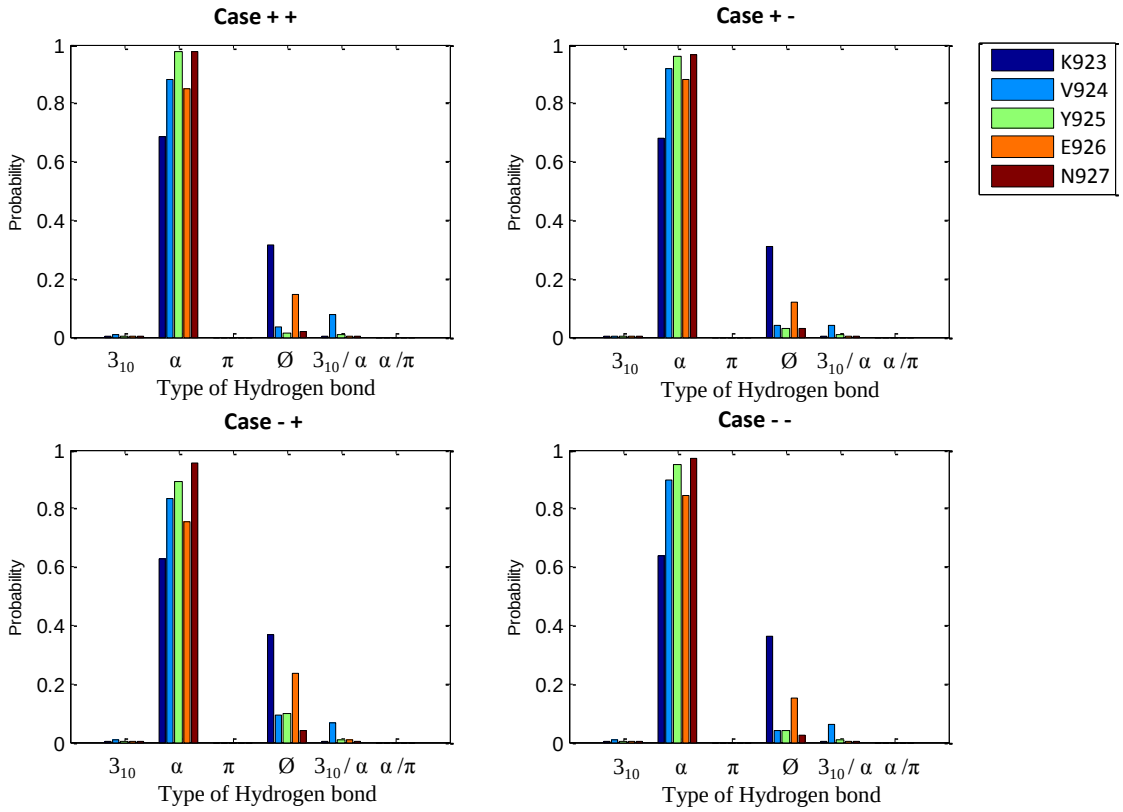


Figure 4-4: Hydrogen bonds types formed in the presence and/or the absence of P1 and P2. H1 primarily forms an α-helix. Each plot represents a cumulative simulation time of 80 ns. (Table 3-1, EQ.WOT.P1P2, EQ.WOT. P1, EQ.WOT.P2, and EQ.WOT.Ø)

Recalling the necessity of H1 to adopt β-strand conformation for making Y925 accessible for phosphorylation, H1 does not have the capacity to accomplish this requirement under only thermal fluctuation.

4.1.1.3 Salt Bridges between H1 Tail and H4

Figure 4-5 shows the wide distribution of the salt bridge distances (SB1: R919-D1039 and SB2: D922-R1042) formed between H1 tail and H4. This wide distribution means that they are not stable and broken most the time. The first salt bridge (SB1) has a wider distribution than the second one (SB2). Even the second salt bridge, with a shorter

range of fluctuation, appears to be broken more often than the first. The reason, why the second salt bridge is broken more often, is because R1042 finds another partner, namely N916, backbone oxygen (Figure 4-6). The first salt bridge has a wide distribution because it is formed between the residue R919, farther inside H1 tail that has more mobility, and residue D1039 in H4.

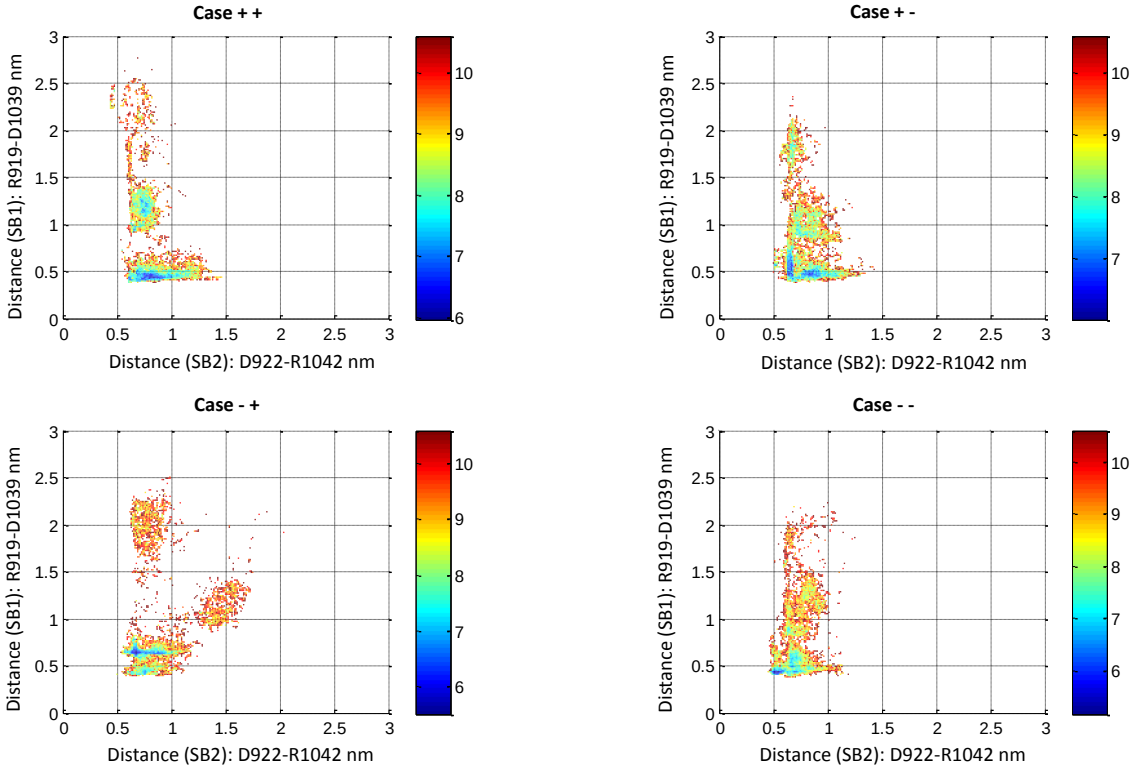


Figure 4-5: Energy landscape of the H1/H4 salt bridge distances represented by SB1 (R919–D1039) and SB2 (D922–R1042). SB1 and SB2 have a wide distribution which means they are broken. This suggests that they are not primarily responsible for keeping H1 folded within the bundle. Each plot represents a cumulative simulation time of 80 ns. (Table 3-1, EQ.WOT.P1P2, EQ.WOT. P1, EQ.WOT.P2, and EQ.WOT.Ø).

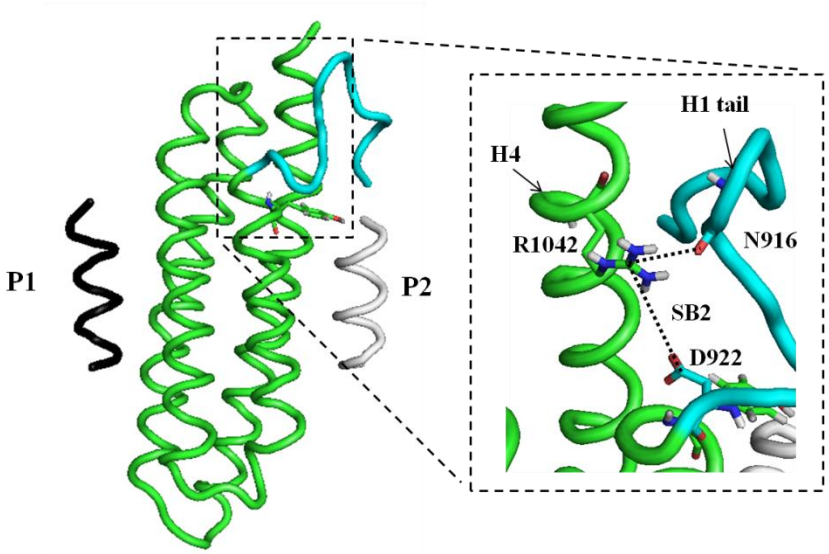


Figure 4-6: The second salt bridge (SB2: D922-R1042) that is located in the region near the N-terminal of H1 (near Y925). The residue R1042 interacts with another partner which is N916.

As seen in Figure 4-7, if the salt bridge distance must be less than 0.5 nm, then the second salt bridge, SB2 (D922–R1042), is broken most the time for any case, whereas the first salt bridge, SB1 (919–D1039), persists 30% of the time. The relative position of H1 tail to the bundle is stable, which makes SB1 persist longer and point the residue, N916, to R1042 closer than D922.

However, it has been suggested that these salt bridges, among other factors, are responsible of maintaining relative position of H1 with the bundle. This result suggests that it does not appear that these salt bridges have a significant role in keeping H1 attached to the bundle.

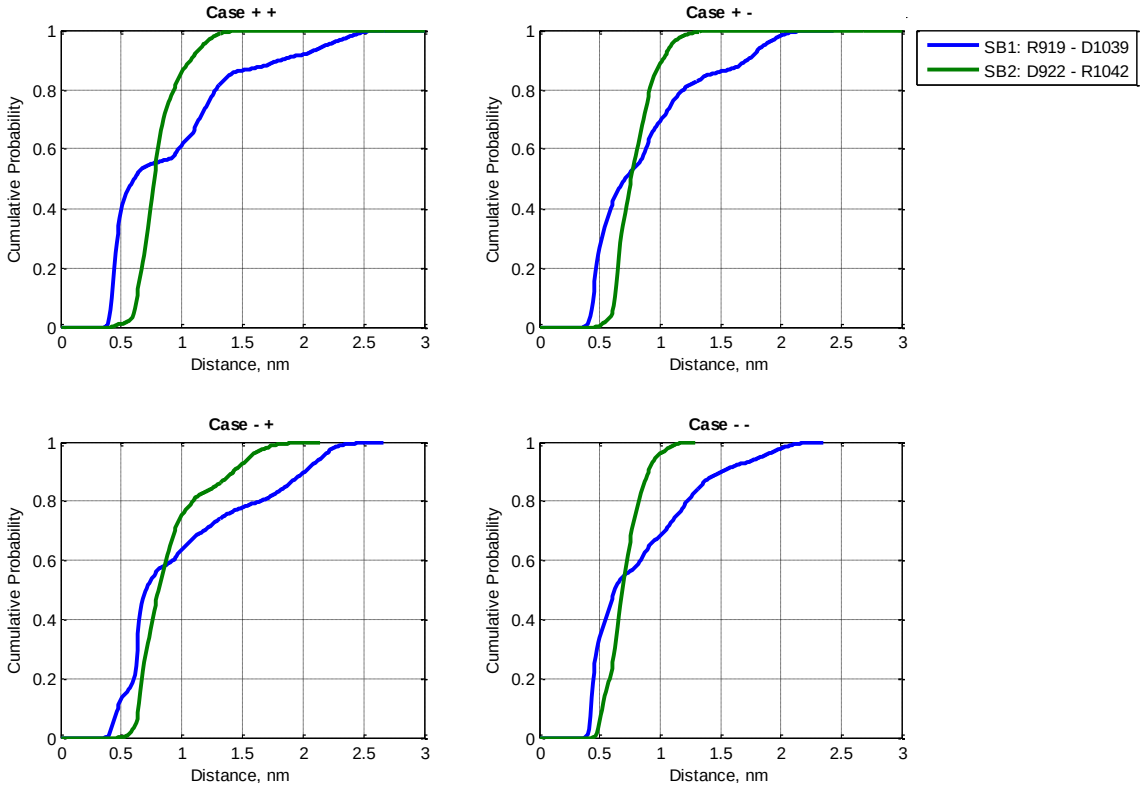


Figure 4-7: Cumulative probability of the two salt bridges represented by two distances SB1 (R919–D1039) and SB2 (D922–R1042). If the salt bridge distance has to be less than 0.5 nm, it means they are broken ~80%. This suggests that they are not primarily responsible for keeping H1 folded within the bundle. Each plot represents a cumulative simulation time of 80 ns. (Table 3-1, EQ.WOT.P1P2, EQ.WOT. P1, EQ.WOT.P2, and EQ.WOT.Ø).

4.1.2 AUGMENTED FAT/PAXILLIN COMPLEX WITH H4 TAIL AND P1/P2 CONSTRAINED

For equilibrium simulations, the augmented FAT/paxillin structure was used and the presence/absence of P2 was varied (Figure 3-4.C and Table 3-1, EQ.WT.P1P2, EQ.WT.P1). This structure was introduced to the mechanically loaded simulation, so understanding its behavior under equilibrium is important. It is very important to examine the effect of the three modifications applied to FAT/paxillin complex of H1 behavior: the

addition H4 tail, the addition of the random coils to P1 and P2, and enforcing a zero displacement condition to the ends of P1 and P2.

4.1.2.1 H1 Position

Figure 4-8 shows the blue colored regions (minima) of H1 position that have small distribution. The relative position of H1 to neighboring helices is very stable which means H1 does not appear to have a propensity to leave the bundle for two simulated cases. In the absence of P2 (binds to HP2), H1 is still attached to the bundle. Moreover, the modifications made to the FAT/paxillin complex do not influence the stability of the position of H1 relative to the bundle. As a result, H1 is strongly attached to the bundle regardless any augmented changes made or the absence of P2.

It seems that under thermal fluctuations only, H1 does not have the ability to overcome the energy barrier, that keeps H1 attached to the bundle. If this is the case, Y925 might not be accessible for the phosphorylation in which H1 has to be out of the bundle

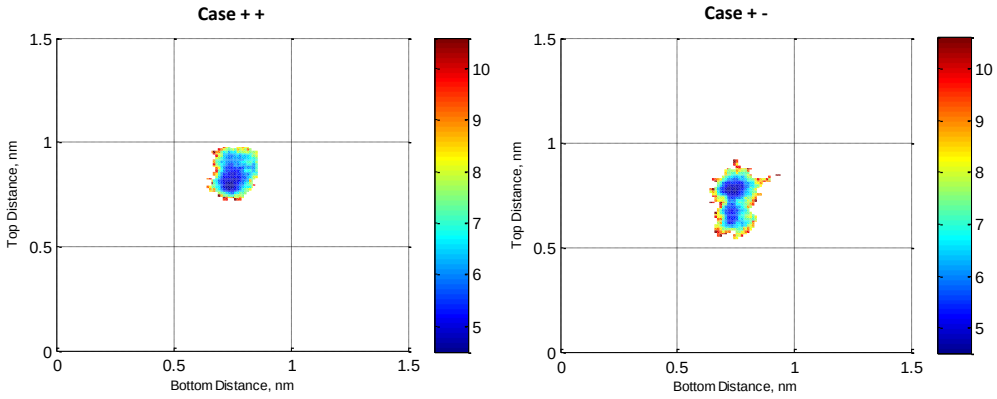


Figure 4-8: Energy landscape of H1 position represented by d_{top} and d_{bottom}. H1 position has a small distribution (minima) which means H1 does not appear to have the propensity to leave the bundle under only thermal fluctuation. Each plot represents a cumulative simulation time of 80 ns. (Table 3-1, EQ.WT.P1P2, EQ.WT. P1).

Figure 4-9 illustrates why the two blue colored regions (minima) for the Case +- exist. They are different stable states in different runs, not different stable states in one simulation. The top distance between H1 and the bundle for Run#1 and Run#4 is slightly smaller than it is in Run#2 and Run#3. After compiling their data in one plot, these two blue spots in Figure 4-8 appeared.

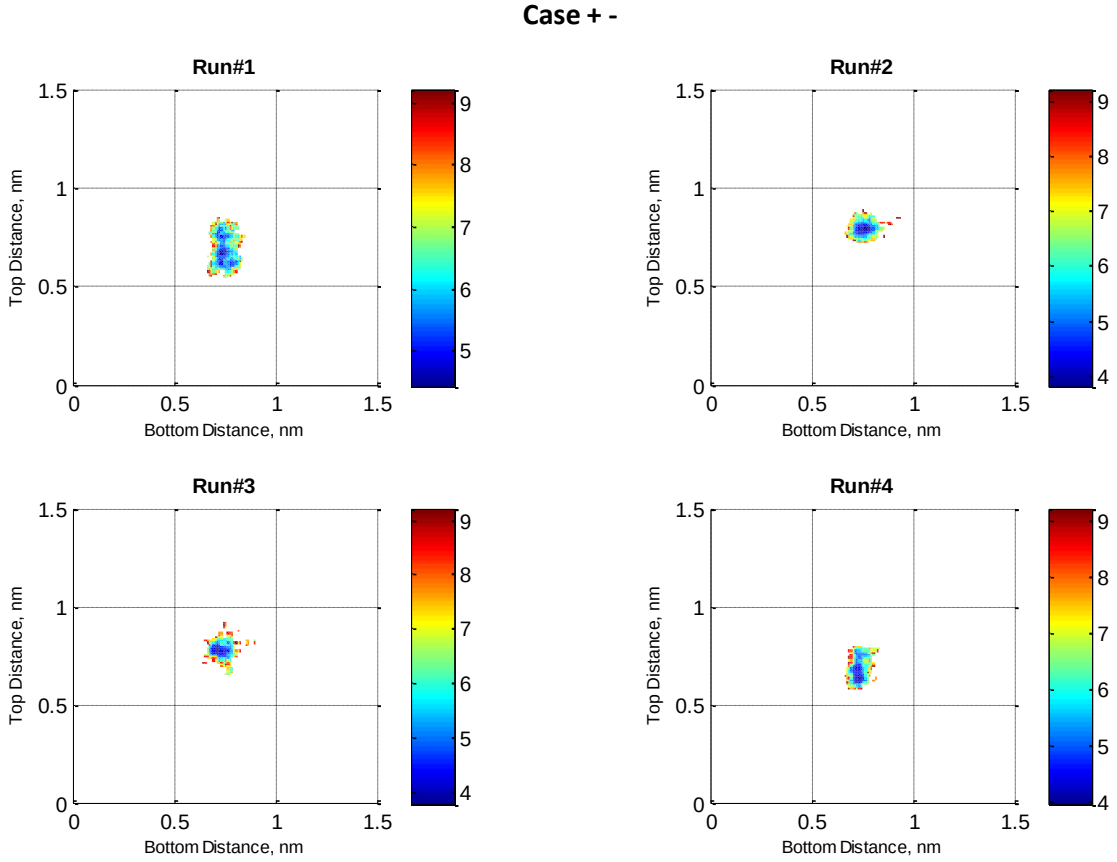


Figure 4-9: Energy landscape of H1 position represented by d_{top} and d_{bottom} in the presence of P1 only. Two different preferred states in different simulations illustrate the presence of the two local minima in the previous figure (Figure 4-9: Case +-). Each plot represents a simulation time of 20 ns. (Table 3-1, EQ.WT. P1).

4.1.2.2 H1 Unfolding

4.1.2.2.1 Backbone Dihedral Angle ψ

As seen in Figure 4-10, except residue K923, the ψ angles of the other top four residues of the H1's N-terminal (V924, Y925, E926, and N927) have a small distribution (the mean value is ~ -50^0 degree). This means they are folded in a helical form in the presence/absence of P2. However, the first residue at the N-terminus of H1 (K923) is expected, as discussed before, to have greater flexibility, since it connects with the H1 tail (i.e., H1 tail is free to move). Even though, the flexibility of K923 does not affect the stability of the other residues flanking Y925. Furthermore, the augmented changes made to the FAT/paxillin structure do not appear to significantly affect the ability of H1 to stay folded. The region flanking Y925 does not appear to have the propensity to adopt β-strand conformation. Even if residue K923 has a propensity to unfold, all other residues are stable and not affected by its flexibility. As a result, H1 does not have the propensity to adopt β-strand conformation under only thermal fluctuation. This means H1 might not have the ability to undergo the structural rearrangements needed for making Y925 accessible for phosphorylation.

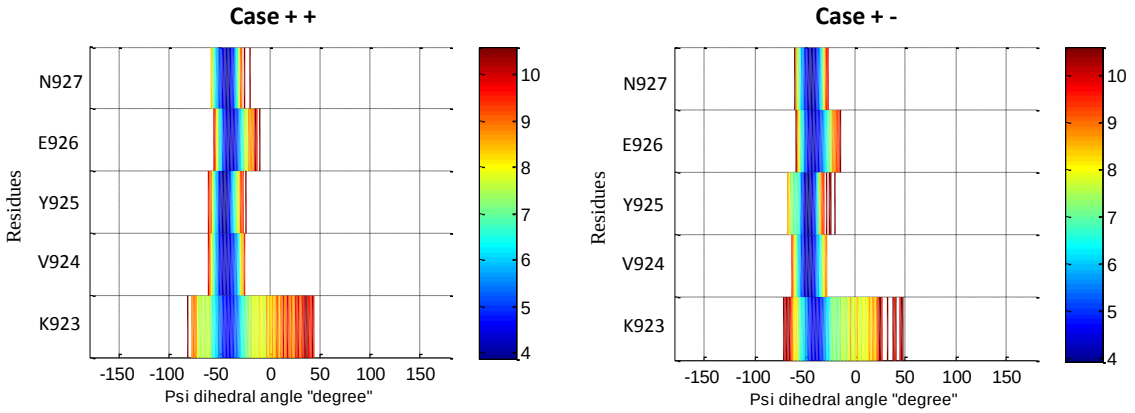


Figure 4-10: Energy landscape of the dihedral angle ψ of the five N-terminal residues of H1 (K923, V924, Y925, E926, and N927) in the presence and the absence of P2. Except K923 that have greater flexibility, since it connects with the floppy tail (H1 tail), ψ angle of other residues have a small distribution (minima). This means H1 does not appear to have the propensity to adopt β-strand conformation under only thermal fluctuation. Each plot represents a cumulative simulation time of 80 ns. (Table 3-1, EQ.WT.P1P2, EQ.WT.P1).

4.1.2.2.1 Hydrogen Donor-Accepter Pairs

Figure 4-11 shows the probability of different types of hydrogen bond formed by the first five residues at the N-terminal of H1 (K923, V924, Y925, E926, and N927). Most the time, they form an α-helix hydrogen bond type. The other hydrogen bond types were formed very rarely. The hydrogen bond of K923 is broken about ~ 30% of the time. However, the hydrogen bonds of other four residues are broken about 3% to 10% of the simulation time. The residue K923 is expected to have more broken hydrogen bond; as discussed before, since it connects to the H1 tail. Examining the propagation of the unfolding, if any, hydrogen donor-acceptor pairs metric is useful. Based on what is shown in Figure 4-11, the unfolding of K923 does not propagate into the other four residues which they are stable. Moreover, the augmented changes made to the FAT/paxillin complex and the absence of P2 do not disrupt H1 α-helical form.

In the presence of P1and P2 (Case ++), the hydrogen bond of the first residue is more likely to be broken than in the absence of P2 (Case +-). This is possibly because the motion constraint that the presence of the constrained P2 provides, but in general, the difference is not significant.

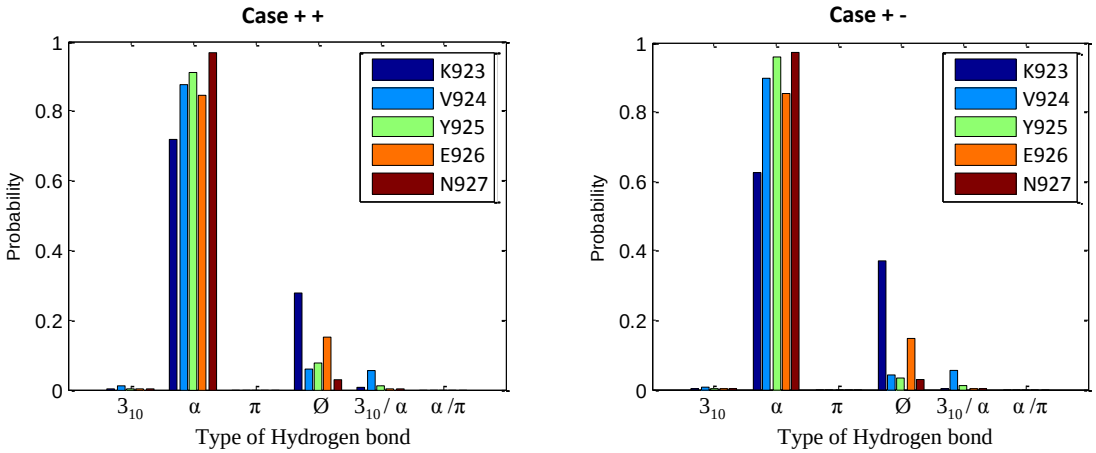


Figure 4-11: Hydrogen bonds types formed in the absence of P2. H1 primarily forms an α-helix. Each plot represents a cumulative simulation time of 80 ns. (Table 3-1, EQ.WT.P1P2, EQ.WT.P1).

4.1.2.3 Salt Bridges between H1 Tail and H4

Figure 4-12 shows the wide distribution of distances between residues formed by the two salt bridges (SB1: R919-D1039, SB2: D922–R1042). This wide distribution means they are broken most the time. For Case +- (in the absence of P2), the first salt bridge (SB1: R919-D1039) has a wider distribution than the second one (SB2: D922–R1042). As discussed before, because R1042 finds another partner N916, backbone oxygen, Figure 4-6, the second salt bridge is broken more. For Case ++ (P1 and P2 are in presence), the first salt bridge has smaller distribution because the relative motion of H1 tail to the bundle is constrained by the presence of P2 (P2 is constrained). In addition, the

augmented changes made to FAT/paxillin structure do not provide supports to these two salt bridges. Their persistence is similar to that found in previous simulations (FAT/paxillin complex without H4 tail and P1/P2 unconstrained, Figure 3-1).

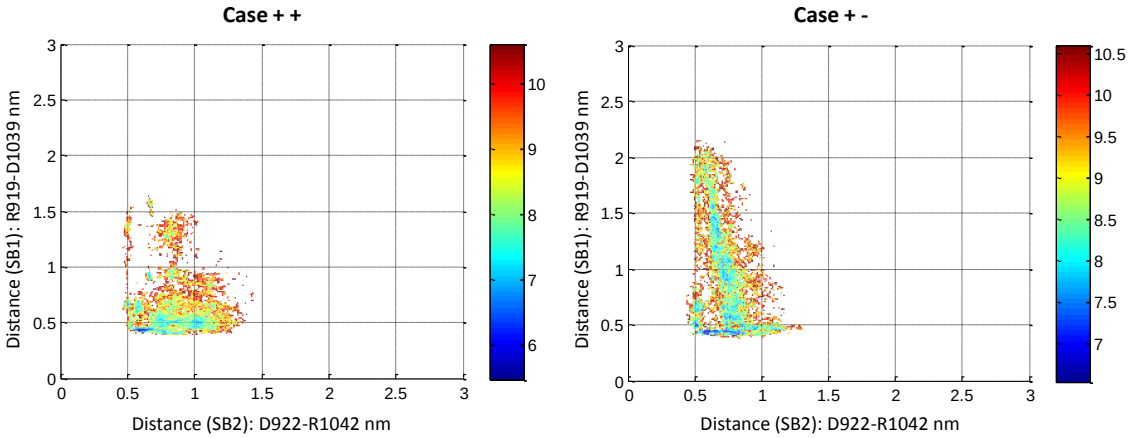


Figure 4-12: Energy landscape of the H1/H4 salt bridge distances represented by SB1 (R919–D1039) and SB2 (D922–R1042). SB1 and SB2 have a wide distribution which means they are broken. This suggests that they are not primarily responsible for keeping H1 folded within the bundle. Each plot represents a cumulative simulation time of 80 ns. (Table 3-1, EQ.WT.P1P2, EQ.WT.P1).

As in Figure 4-13, if the salt bridge distance must be less than 0.5 nm, then the second salt bridge, SB2: D922–R1042, is broken most the time for any simulated case, whereas the first one persists 20~40% of the time. Besides other factors, the two salt bridges between H1 and H4 are often cited as being responsible for keeping H1 attached to the bundle. However, these results show the opposite: they are not stable, which means they might not have a significant contribution in holding H1 to the bundle.

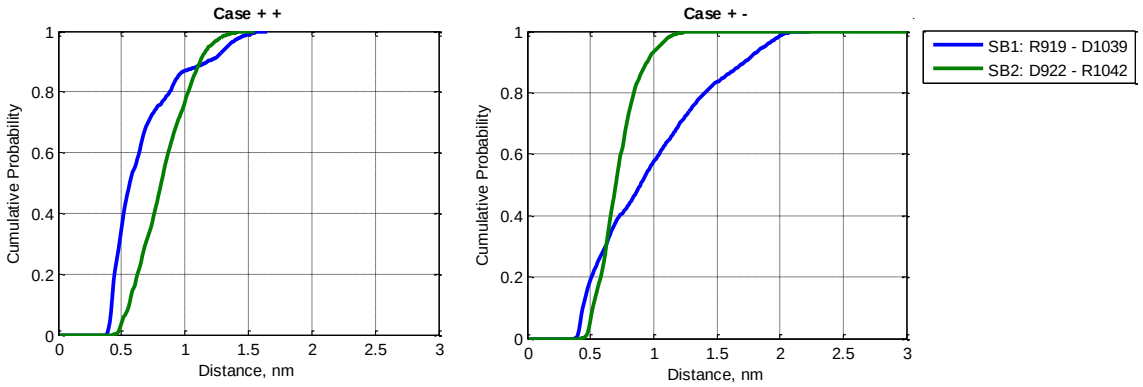


Figure 4-13: Cumulative probability of the two salt bridges represented for two distances, SB1 (R919–D1039) and SB2 (D922–R1042). If the salt bridge distance has to be less than 0.5 nm, it means they are broken ~80% of the simulation time. This suggests that they are not primarily responsible for keeping H1 folded within the bundle. Each plot represents a cumulative simulation time of 80 ns. (Table 3-1, EQ.WT.P1P2, EQ.WT.P1).

4.1.3 H1 ISOLATION

Previous results suggest that H1 prefers to stay folded in an α-helical form within the bundle. In addition, the two salt bridges are broken most often and they do not appear to be the key of holding H1 to the bundle. There must, therefore, along with the hydrogen bonds, be another factor contributing to maintaining the helical form of H1, as well as holding it to the bundle. Therefore, it is important to consider the possible effect of the hydrophobicity of the FAT domain core on H1 and examine the H1 behavior as it is isolated.

Figure 4-14 shows H1 behavior under two types of simulations: A) MD for the entire FAT system, and B) MD for H1 isolated from FAT. H1 stays in a helical form as it attached to the bundle and it unfolds when it is isolated. Even though, H1 started to unfold from its C-terminal (where the H1/H2 hinge connects to) while the region flanking Y925 at the N-terminal struggled for long time in keeping its helical form. This illustrates the influence of the hydrophobicity of the FAT core on H1, as well as the propensity of H1 to unfold from its C-terminal. It has been suggested that this hinge between H1 and

H2 has the ability to promote such an unfolding transition to the H1 helix. This results are consistent with both the important role of the hydrophobicity on H1 behavior, as well as the propensity of H1 to unfold from its C-terminal (where Y925 is located at N-terminal portion).

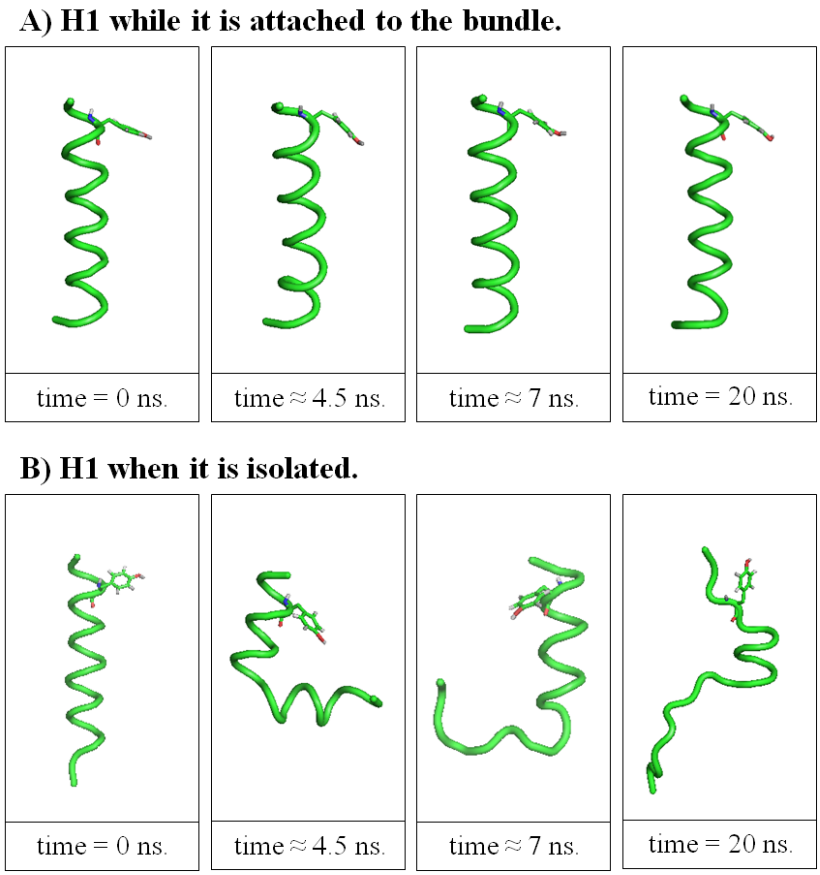


Figure 4-14: The structural conformation of H1 under two conditions; H1 within the bundle and H1 isolated. A) H1 while it is attached to the bundle (Figure 3-1). It shows that H1 has the ability to keep its in helical form when it is associated with the bundle. B) H1 when it is isolated (K923-K941). H1 has a propensity to unfold from its C-terminal.

4.1.4 PAXILLIN LD MOTIF ISOLATION

To examine the assumption that suggests LD motif is α-helix in its native form, MD simulation was run for an isolated LD4 motif. Figure 4-15 shows LD4 behavior under two type of simulation: LD motif when it is isolated, LD motif bound to the FAT

domain. When isolated, the LD motif unfolded in 2 ns which means that LD motif does not appear to have the ability maintain its helical form by itself. However, when LD motif binds to the FAT domain, it stays in a helical form. This contradicts what is stated in the literature and illustrates the role of hydrophobicity of the hydrophobic patches HP1 and HP2 on the conformational structure of the LD motifs as they associate with the FAT domain. It does not seem that LD motifs stabilize the bundle form of the FAT domain, but the FAT domain has the capacity to stabilize the helical form of LD motifs when they are in association.

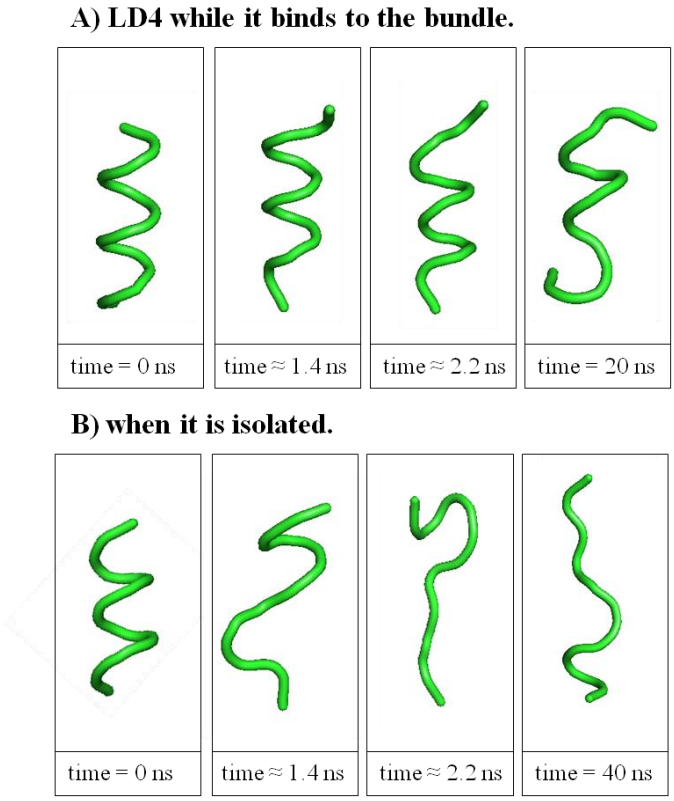


Figure 4-15: The structural conformation of LD4 under two conditions; LD4 binds to FAT domain and LD4 isolated. A) Snapshots for LD motif while it binds to the FAT domain (Figure 3-1). It shows that LD motif has the ability to keep its in helical form when it is associated with the bundle. B) Snapshots for LD motif when it is isolated (T264-S275). The isolated LD does not have the capability to stay folded, which illustrates the effect of the hydrophobic patches that LD binds to.

4.1.5 EQUILIBRIUM RESULT SUMMARY

The total time of equilibrium simulations, 560 ns, was run for different cases (in the presence/absence of P1 and P2) and different structure (FAT/paxillin complex without H4 tail and P1/P2 unconstrained, and augmented FAT/paxillin complex with H4 tail and P1/P2 constrained). For all these equilibrium simulations, H1 position metric strongly suggests that independent of binding to the paxillin, H1 does not have the propensity to leave the bundle under only thermal fluctuation. In addition, H1 unfolding metrics suggest that H1 stays folded in α-helical form. In the case where H1 is isolated, H1 has the propensity to unfold from its C-terminal (not from the N-terminal where the Y925 is located). This result is consistent with what has been suggested in the literature about the energy barrier that prevents H1 to leave the bundle. However, the two reported salt bridges (SB1: R919-D1039, SB2: D922–R1042) were weak and not able to persist, which contradicts what stated in the literature that these salt brides have a role in holding H1 to the bundle.

As discussed before, it has been suggested for Y925, which isolated at the N-terminal of H1, to be accessible for phosphorylation, H1 has to come out of the bundle and adopt a β-strand conformation. Whereas under only thermal fluctuation, it does not appear that the FAT domain is able to undergo the required structural rearrangements needed for phosphorylation. This suggests that under only thermal fluctuation, Y925 is not frequently accessible for phosphorylation. Moreover, the salt bridges metric raises a question of the ability of the interactions, observed from the crystal structure of a protein, to persist in the dynamic in vivo environment.

For Y925 to be accessible for phosphorylation, mechanical loads or/and chemical interaction(s) have to take place to promote the required structural changes. From

mechanical standpoint, the FAK has been hypothesized to be mechanically activated. The next section presents results of H1 behavior under applied load.

4.2 Loaded Scenario Results

As discussed in the equilibrium results, the thermal fluctuation does not appear to have the capacity to promote the required structural rearrangement of the FAT domain needed for making Y925 accessible for the phosphorylation. H1 neither leaves the bundle nor adopts a β-strand conformation under only thermal fluctuation. As a result, axial and perpendicular mechanical loaded simulations were run (illustrated in §3.2.4 Simulations). The H1 behavior, in terms of its relative position and unfolding, under the influence of the load was examined using Constant Force Molecular Dynamics (CFMD) simulations on as many different initial structures as possible (discussed in §3.1.1 Simulations).

4.2.1 AXIAL LOAD SCENARIO RESULTS

Five different initial structures (seeds, Figure 3-9) were chosen based on the behavior of H1/H4 tail, their relative position to each other as well as how many interactions they have (Figure 3-8). Each seed was run twice, with different initial velocities (Table 3-1, AX.WT.P1P2). A 100 pN constant force is applied to the N-terminus of H1 tail in a direction parallel to the H1 axis with P1/P2 were constrained. The results of the axial load simulation show two types of H1 behavior: typical and atypical (Table 4-1).

Table 4-1: H1 typical and atypical behaviors under axial load, applied to the N-terminus of H1 tail and P1/P2 constrained. Eight out of ten simulations have typical behavior, while two have atypical behavior. (Table 3-1, AX.WT. P1P2).

Initial Structures		H1 Behavior Type		H1 Behavior Description	
		Typical	Atypical	H1 Position	H1 Unfolding
Seed#1	Run#1	Yes	-	In the bundle	In a helical form
	Run#2	Yes	-	In the bundle	In a helical form
Seed#2	Run#1	Yes	-	In the bundle	In a helical form
	Run#2	-	Yes	In the bundle	The first two residues, K923 and V924, of H1 unfold.
Seed#3	Run#1	Yes	-	In the bundle	In a helical form
	Run#2	Yes	-	In the bundle	In a helical form
Seed#4	Run#1	Yes	-	In the bundle	In a helical form
	Run#2	Yes	-	In the bundle	In a helical form
Seed#5	Run#1	-	Yes	In the bundle	The first two residues, K923 and V924, of H1 unfold.
	Run#2	Yes	-	In the bundle	In a helical form

4.2.1.1 H1 Typical Behavior

Eight simulations out of ten have the same H1 behavior (Table 4-1). These eight simulations started with different initial conditions (seeds and initial velocities). Regardless the differences in their initial conditions, the behavior of H1 is very similar. The typical behavior of H1 is similar to its behavior under equilibrium.

4.2.1.1.1 H1 Position

As seen in Figure 4-16, the blue-colored regions (minima) of the H1 position have small distribution. For all the different initial conditions applied, the relative position of H1 to the bundle is very stable, which means H1 does not appear to have a propensity to leave the bundle. As suggested in literature, electrostatic and hydrophobic interactions between H1 (residues A917-D922) and H4 present an energy barrier keeping H1 attached to the bundle. A 100 pN constant load applied does not appear to have the ability to overcome this energy barrier. Under equilibrium and axial load, FAT domain moves as a rigid body and the 100 pN axial load does not have the capacity to open the FAT domain. However, in order for Y925 to engage the physphorylation, H1 has to leave the bundle. It seems that Y925 is not easily accessible for phosphorylation.

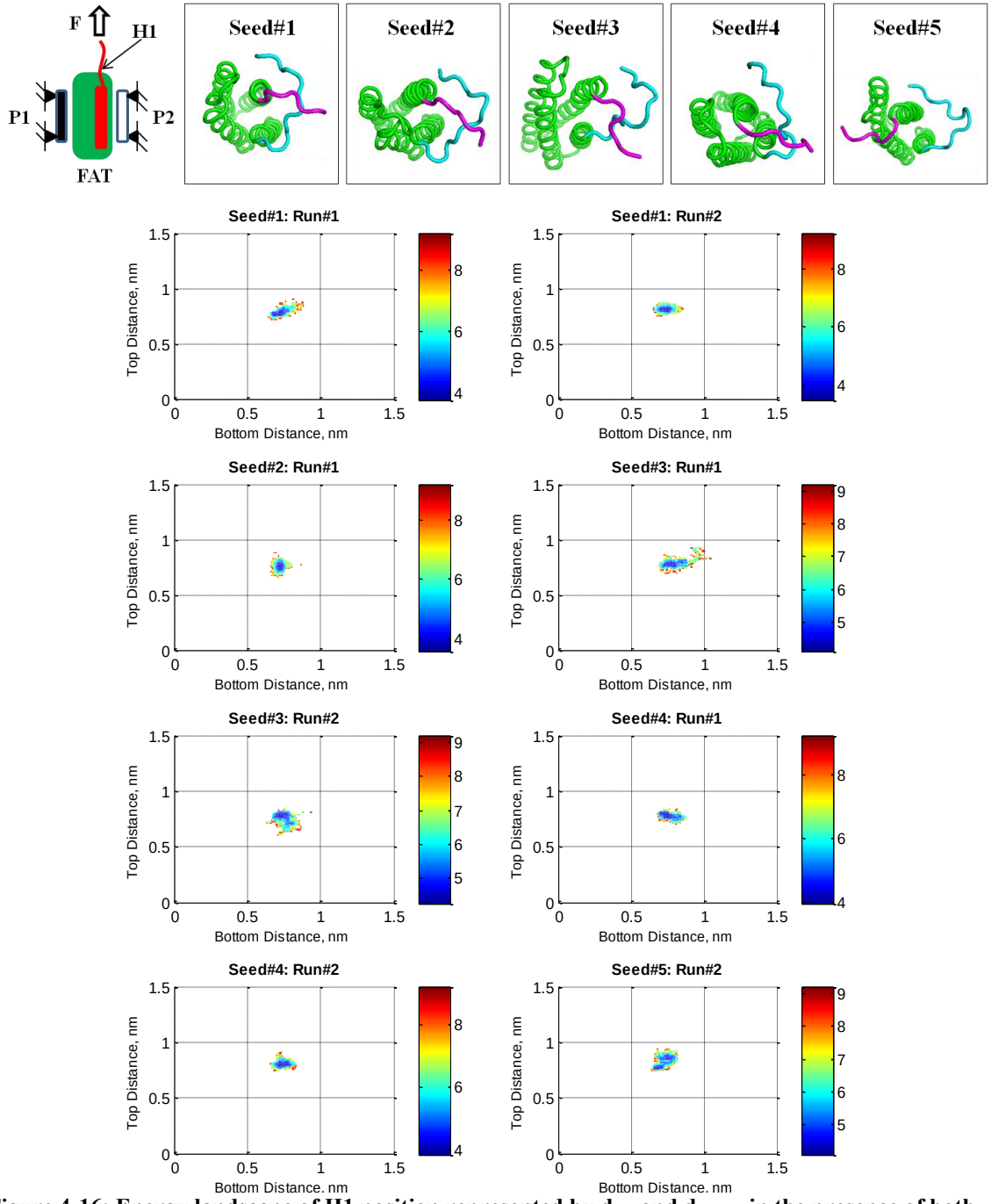


Figure 4-16: Energy landscape of H1 position represented by d_{top} and d_{bottom} in the presence of both P1 and P2. For typical behavior, H1 position has a small distribution (minima) which means H1 does not appear to have the propensity to leave the bundle under constant force applied axially to the N-terminus of H1 tail. Each plot represents a simulation time of 20 ns. (Table 3-1, AX.WT.P1P2).

4.2.1.1.2 H1 Unfolding

4.2.1.1.2.1 Backbone Dihedral Angle ψ

From Figure 4-17, except residue K923, the ψ angles of the other top four residues of the H1's N-terminal (V924, Y925, E926, and N927) have a small distribution (the mean value is ~ -50^0 degree). This means they are folded in a helical form. However, the first residue at the N-terminus of H1 (K923) is expected, as discussed before, to have a greater flexibility, since it connects with H1 tail (i.e., H1 tail is free to move). The flexibility of K923 does not affect the stability of the other residues flanking Y925.

Under equilibrium and an applied 100 pN axial load, the region flanking Y925 does not appear to have the propensity to adopt β-strand conformation. Even when residue K923 has a propensity to unfold, all other residues are stable and not affected by its flexibility. This means H1 has a high resistance to any structural rearrangements needed for making Y925 accessible for phosphorylation.

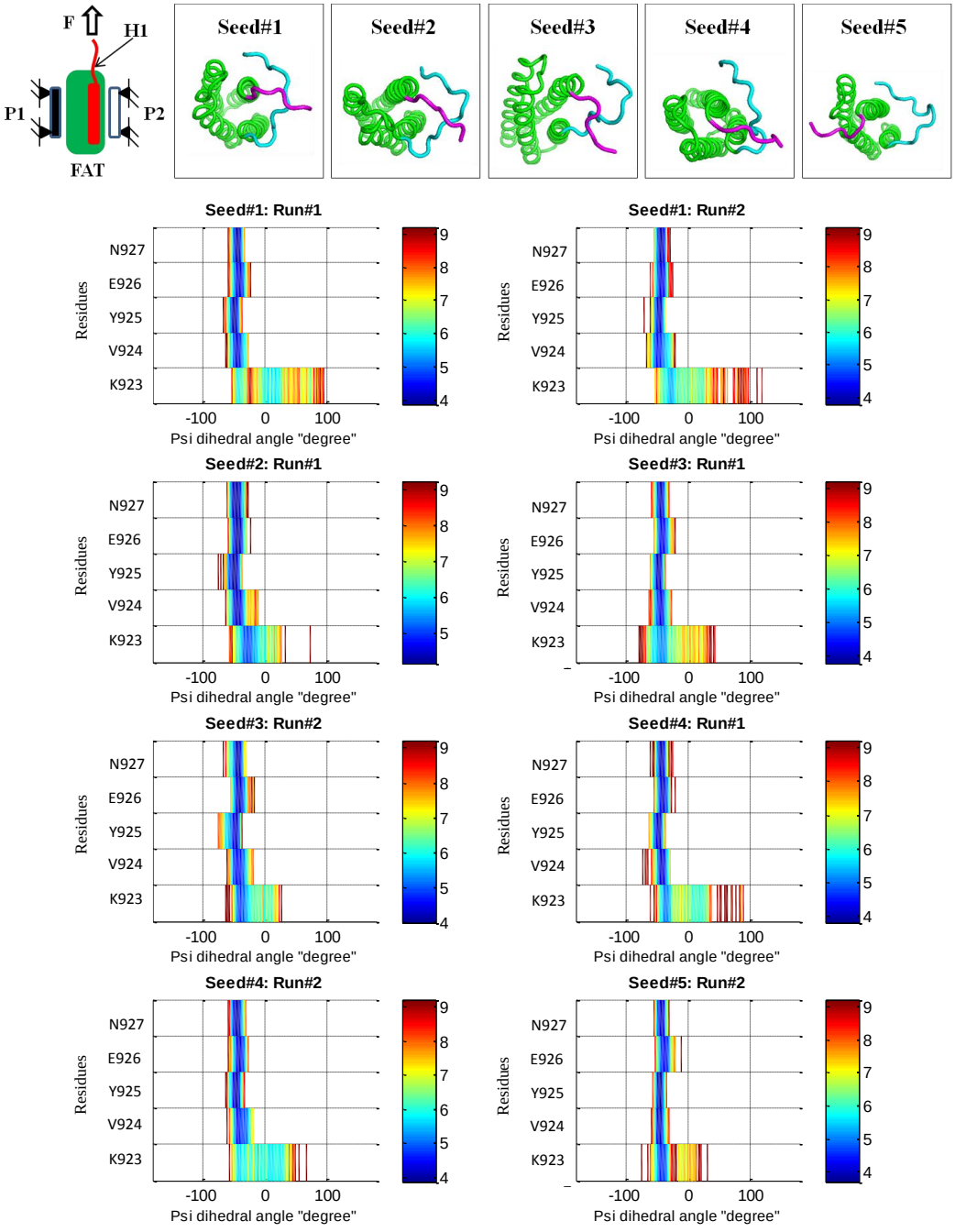


Figure 4-17: Energy landscape of the dihedral angle ψ of the five N-terminal residues of H1 (K923, V924, Y925, E926, and N927) in the presence of both P1 and P2 for H1 typical behavior. Except N923 that has greater flexibility, since it connects with the floppy tail (H1 tail), ψ angle of other residues have a small distribution (minima). This means H1 does not appear to have the propensity to adopt β-strand conformation under constant force applied axially to the N-terminus of H1 tail. Each plot represents a simulation time of 20 ns. (Table 3-1, AX.WT.P1P2).

4.2.1.1.2.2 Hydrogen Donor-Accepter Pairs

Figure 4-18 shows the probability of different hydrogen bond types formed by the first five residues at the N-terminal of H1 (K923, V924, Y925, E926, and N927). Most the time, they form an α-helix hydrogen bond type for any different initial conditions applied. The π and 3_{10}-helix hydrogen bond type formed very rarely. The hydrogen bond of K923 is broken about ~ 50% of the time. However, the hydrogen bonds of other four residues are broken about 3% to 7% of the time. The residue K923 is expected to have more broken hydrogen bond since it connects to the H1 tail.

Hydrogen donor-acceptor pairs metric is useful in examining the propagation of the unfolding, if any. Based on what Figure 4-18 shows, the unfolding of K923 does not propagate into the other four residues where they are stable. Neither thermal fluctuation nor 100 pN axial load appear to excite the region flanking Y925 and promote the needed conformational rearrangements for the phosphorylation.

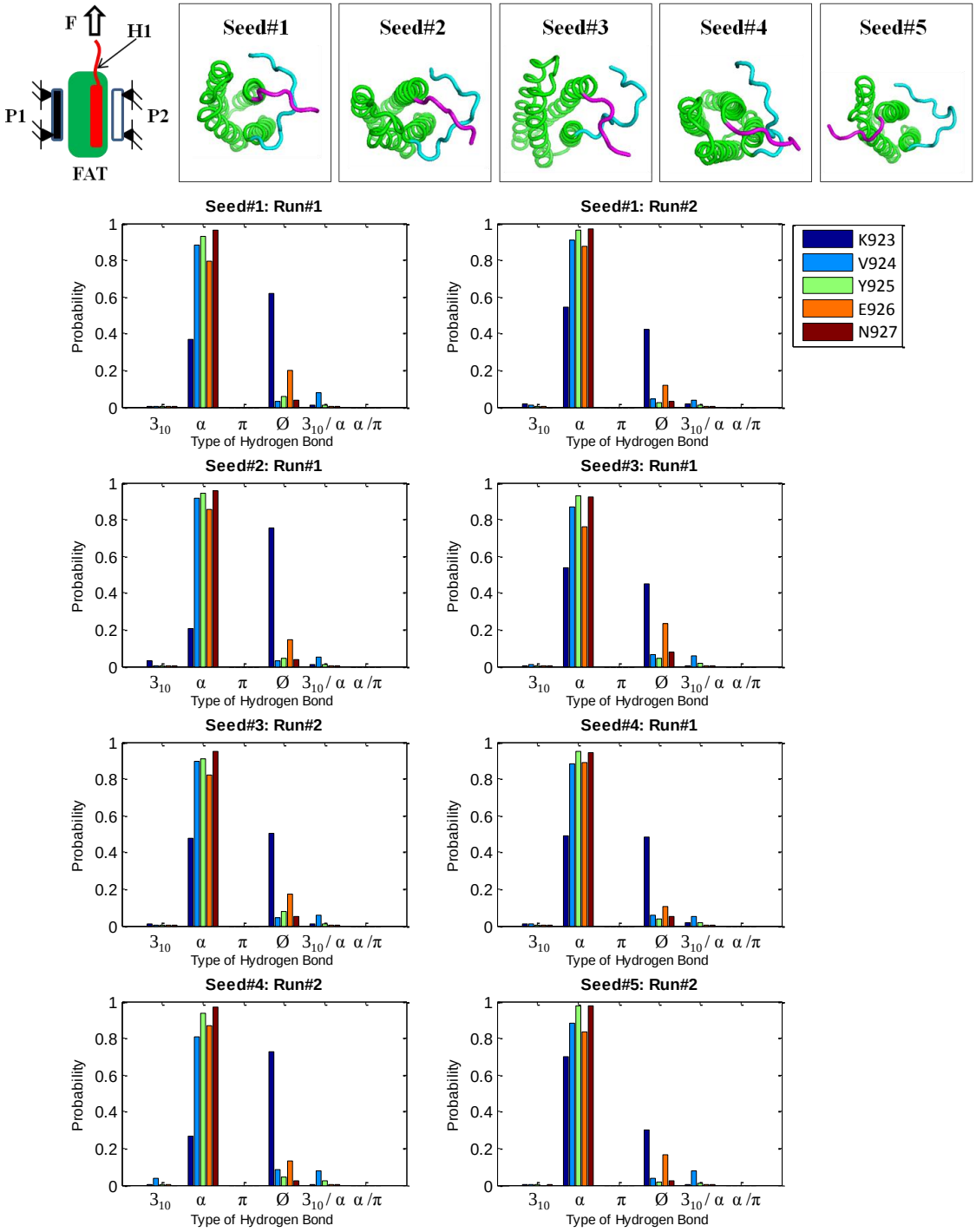


Figure 4-18: Hydrogen bonds types formed in the absence of P2. For H1 typical behavior, H1 primarily forms an α-helix. Each plot represents a simulation time of 20 ns. (Table 3-1, AX.WT.P1P2).

4.2.1.1.3 Salt Bridges between H1 Tail and H4

Figure 4-19 shows the wide distribution of distances between residues that formed the two salt bridges (SB1: R919-D1039, SB2: D922–R1042). This wide distribution of the distance means they are broken most the time. The first salt bridge (SB1) has a wider distribution than the second one (SB2), which is because of the load applied to H1 tail. The H1 tail is pulled in the load direction breaking the first salt bridge more often and pulling the residue, N916, that sometime interacts with R1042, which leads to making the second salt bridge more stable. (Figure 4-20). The applied load makes the first salt bridge weaker and the second salt bridge stronger.

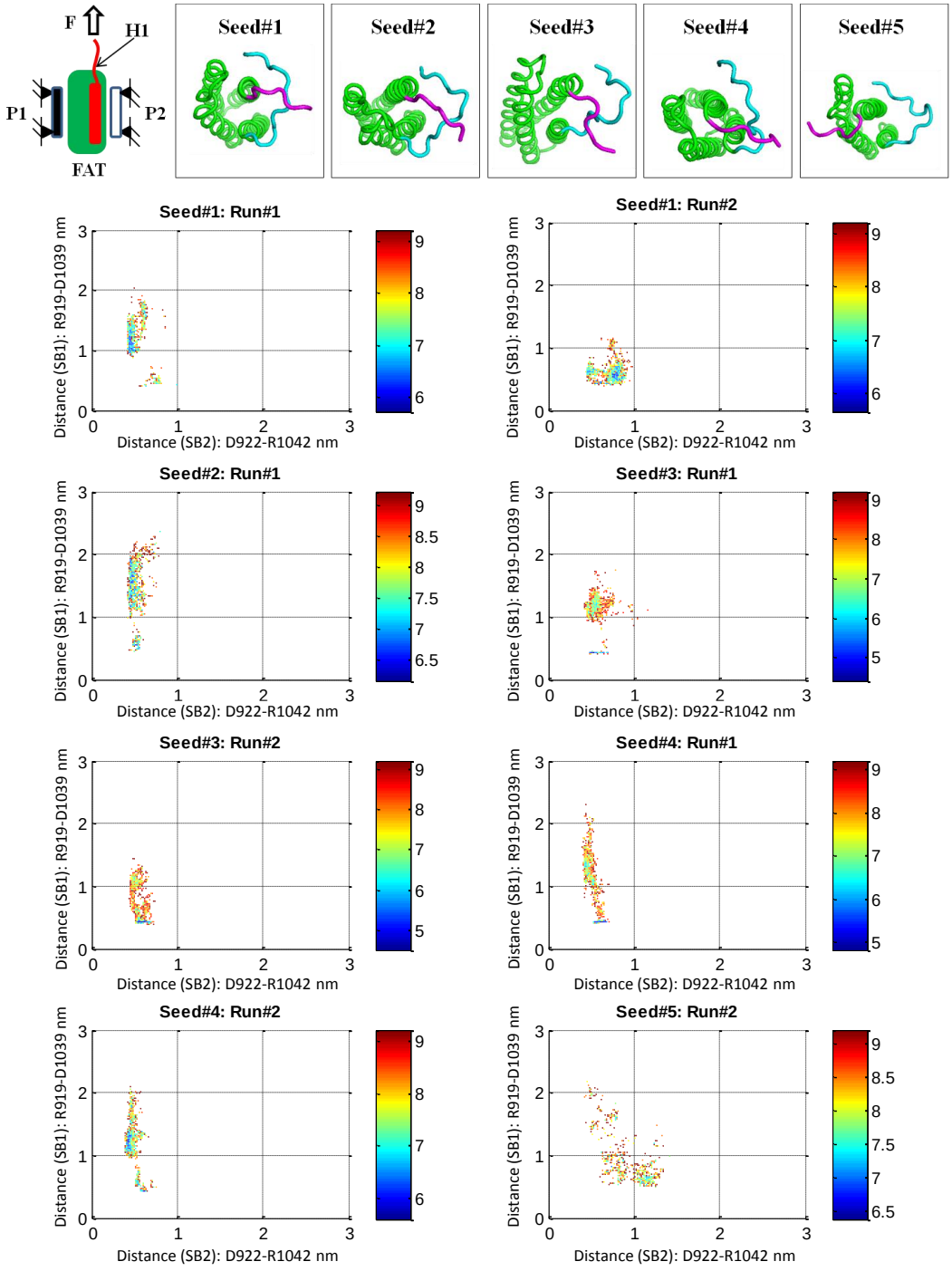


Figure 4-19: Energy landscape of the H1/H4 salt bridge distances represented by SB1 (R919–D1039) and SB2 (D922–R1042). SB1 and SB2 have a wide distribution which means they are broken. This suggests that they are not primarily responsible for keeping H1 folded within the bundle. Each plot represents a simulation time of 20 ns. (Table 3-1, AX.WT.P1P2).

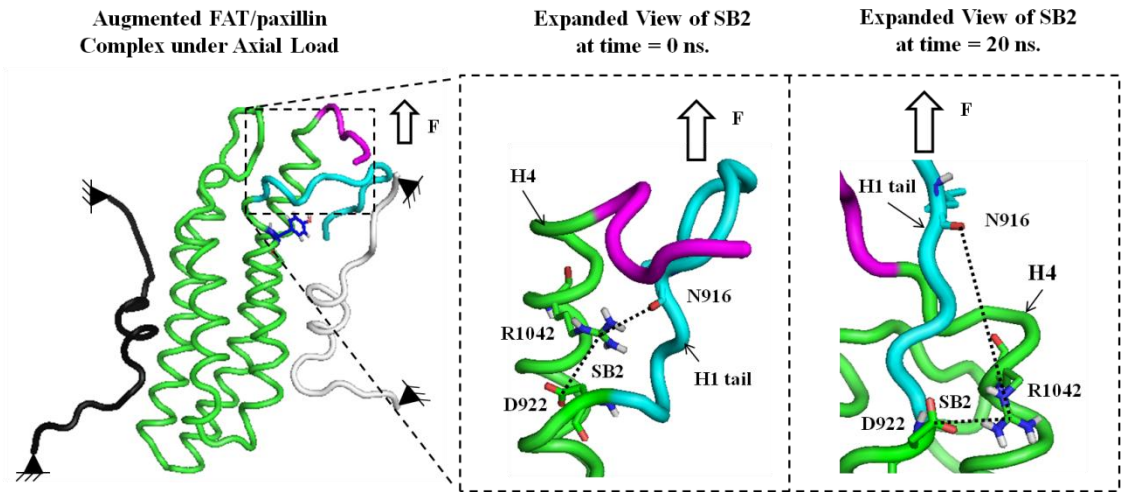


Figure 4-20: The second salt bridge (SB2: D922-R1042) that is located in the region near the N-terminal of H1 (near Y925). The second salt bridge is shown before the simulation started and after. The load applied to the N-terminus of H1 tail pulled N916 away from R1042 making the second salt bridge more stable.

As in Figure 4-21, if the salt bridge distance must be less than 0.5 nm, then the first salt bridge, SB1: D922–R1042, is broken most the time, whereas the second one, SB2: R919–D1039, persists 30% of the time. Under the influence of the axial load, the relative position of H1 tail to the bundle increases, which makes the first salt bridge broken more and pointing the residue, D922, to R1042 closer than N916 (Figure 4-20).

However, it has been suggested that these salt bridges, among other factors, are responsible of maintaining relative position of H1 with the bundle. This result suggests that it does not appear that these salt bridges have a significant role in keeping H1 attached to the bundle. In addition, salt bridge metric suggests that the strength of the interactions between the residues are affected by the applied load.

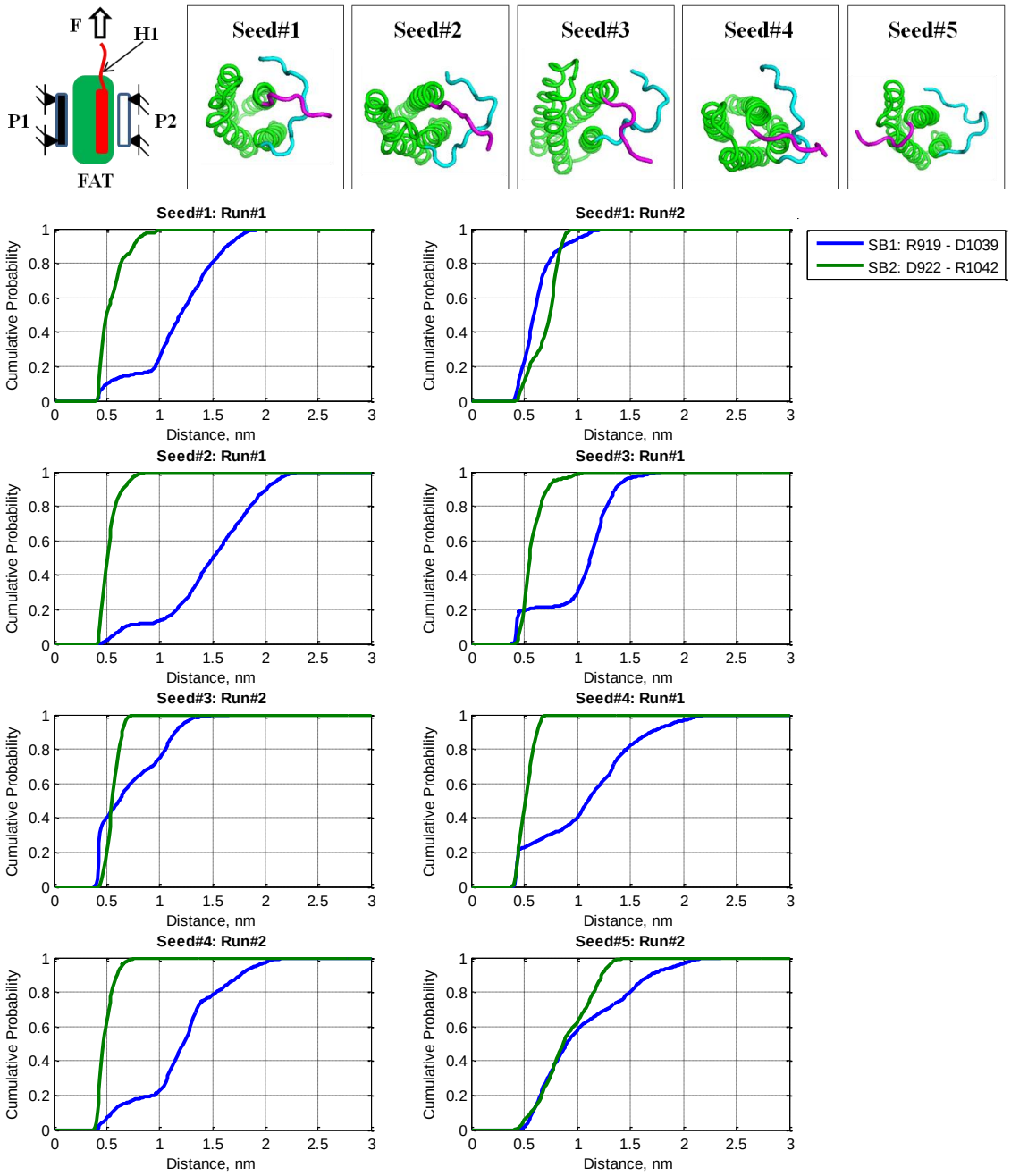


Figure 4-21: Cumulative probability of the two salt bridges represented for two distances, SB1 (R919–D1039) and SB2 (D922–R1042). If the salt bridge distance has to be less than 0.5 nm, it means they are broken ~60%. This suggests that they are not primarily responsible for keeping H1 folded within the bundle. Each plot represents a simulation time of 20 ns. (Table 3-1, AX.WT.P1P2).

4.2.1.1.4 H1/H4 Tail Interaction

Figure 4-22 shows the quality of interactions formed between the H1/H4 tail. The number of H1/H4 tail interactions is widely distributed, the Seed#2 Run#1 and Seed#5 Run#2 are different than the other. In Seed#5 Run#2, H1/H4 tail have mostly no interactions, where the initial structure has no interaction between H1/H4 tail and they are separated. In Seed#2 Run#1, they have 1~3 electrostatic interactions while in other simulations, H1/H4 tail prefers to be entangled through 4 ~7 electrostatic interaction. In Seed#5 Run#2, the two salt bridges are broken and H1/H4 tail are separate, yet H1 is strongly attached to the bundle in a helical form. This suggests that they are another factors that holding H1 to the bundle. (discussed in § 4.2.1.3 Axial Load Result Summary)

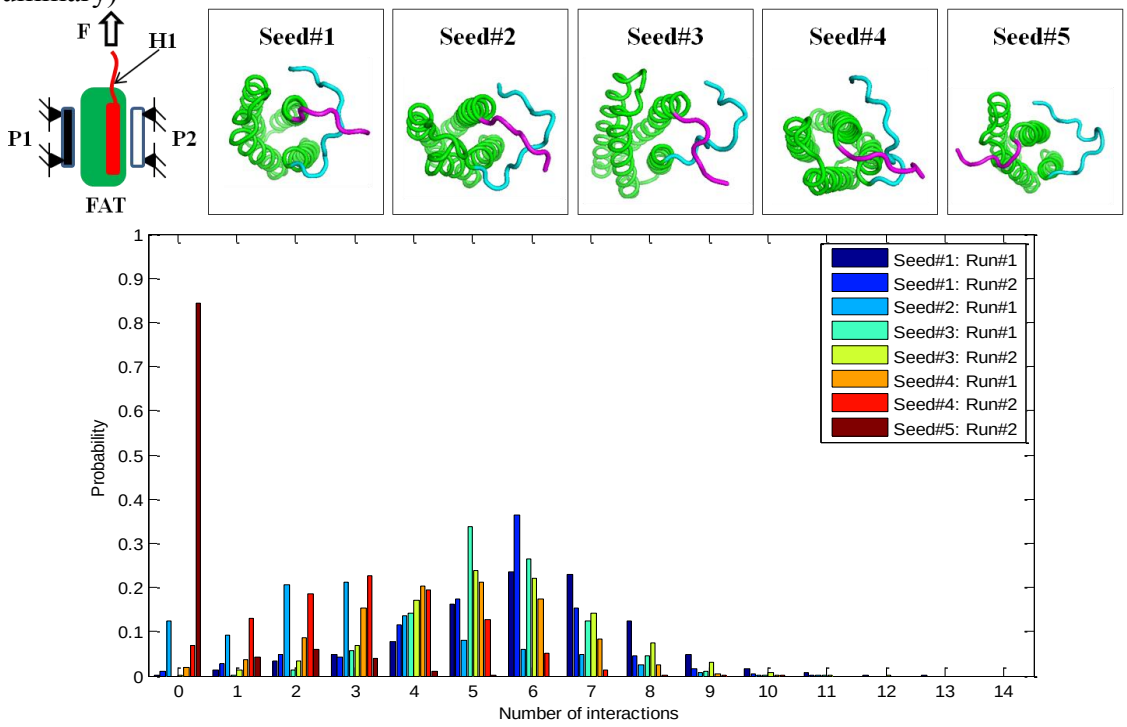


Figure 4-22: Number electrostatic interactions formed between H1/H4 tail. The interactions between H1/H4 have a wide distribution which means H1/H4 tail prefer to entangled. Each bar represents a simulation time of 20 ns. (Table 3-1, AX.WT.P1P2).

4.2.1.1.5 FAT Structure in its Final States

Table 4-2 and Figure 4-23 show the FAT structure's final states in terms of H position, H1 unfolding, H1/H4 tail interactions and H2-H3 structure. In 100% of the eight simulations, H1 stays folded in the bundle. In 50% of the simulations, H1/H4 tail form β-sheet via a number of hydrogen bonds. About 37%, they are entangled via number of electrostatic interactions. This suggests that H1/H4 tail prefer to interact with each other more often. In only one simulation (Seed#5 Run#2), H1/H4 tail are mostly separate. (H1/H4 tail interactions are listed in (Appendix D). In this simulation, H1 stays folded in the bundle, which suggests that H1/H4 tail does not appear to be the key regulator of resisting H1 unfolding or keeping H1 attached to the bundle.

Table 4-2: Final state of the structure of the region flanking Y925 for H1 typical behavior under constant force applied axially to the N-terminus of H1 tail. (Table 3-1, AX.WT.P1P2).

	H1 Position		H1 Unfolding			H1/H4 Tail Interactions				H2-H3 Structure	
	In	Out	F	SUF	UN	β, EX	β, NEX	τ	S	F23	U23
Probability %	8/8	0/8	8/8	0/8	0/8	1/8	3/8	3/8	1/8	6/8	2/8

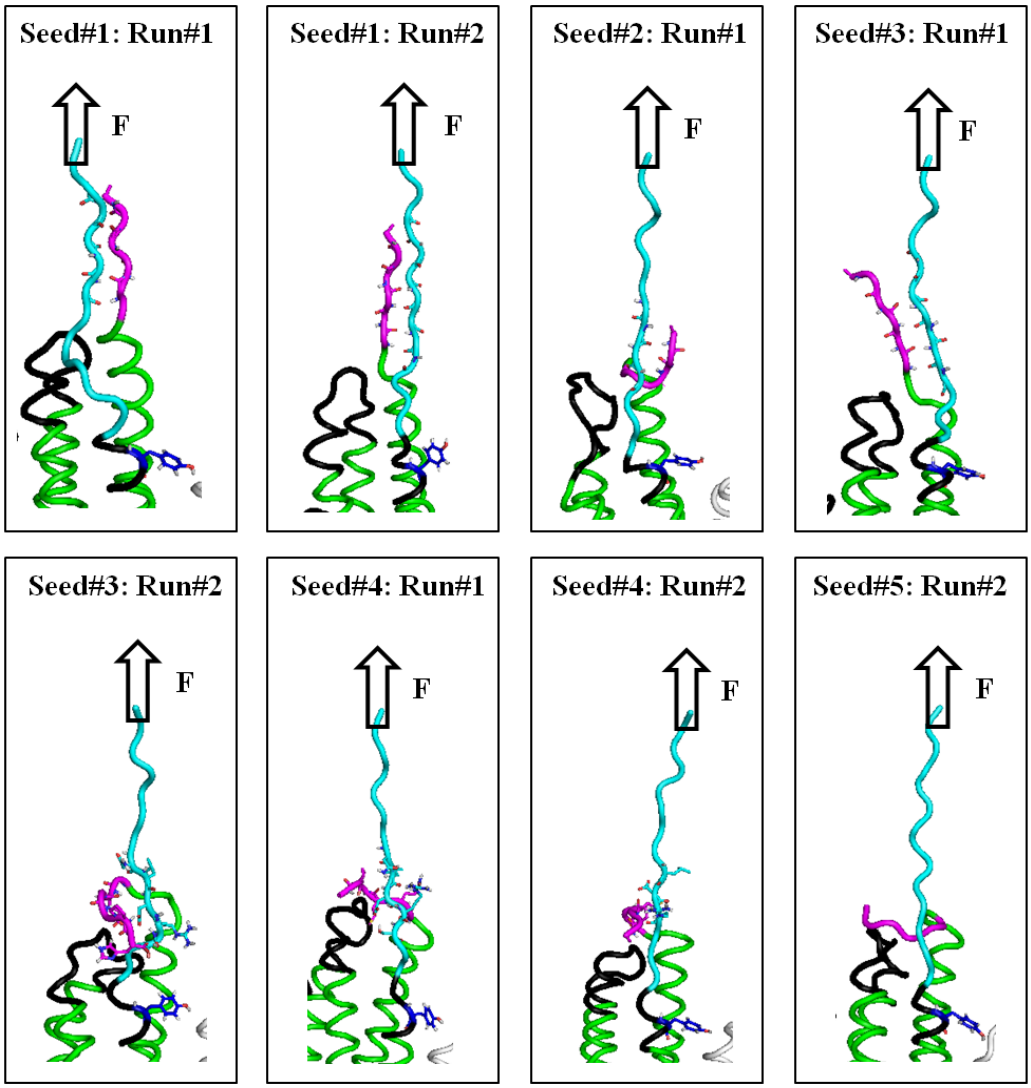


Figure 4-23: Final state of the structure of the region flanking Y925 for H1 typical behavior under constant force applied axially to the N-terminus of H1 tail. (Table 3-1, AX.WT.P1P2).

4.2.1.2 H1 Atypical Behavior

The two other runs out of ten show different behavior of H1 (Table 4-1). They start with different initial structures (Seed#2 and Seed#5). In Seed#2, the H1/H4 tail interact with each other, while in Seed#5, they are separate.

In Figure 4-24, there are four different metrics: H1 position, dihedral angle ψ, hydrogen state and salt bridge state. For both simulations, the relative position of H1 has a small distribution (blue colored region) which means H1 is attached to the bundle. Also, the ψ angle of the second residue of H1's N-terminal (V924) shows that it unfolds. The residue (V924) has more broken hydrogen bond. The hydrogen bond metric shows that the unfolding of the first residue of H1 (K923) propagates into only the second residue (V924) where the other residues are stable. In addition, in Seed#5, Run#1, the second salt bridge (D922-R1042) is broken more often than the one in the Seed#2, Run#2. However, the first salt bridge (R919-D1039) is broken most the time.

In general, even the first two residues of N-terminal of H1 unfold, their unfolding do not propagate into the H1 helix to create β-strand conformation. Moreover, even these two residues show a propensity to unfold, H1 does not appear to have the capacity to leave the bundle. This atypical behavior of H1 does not achieve the required structural changes needed for Y925 phosphorylation, where H1 must leave the bundle and adopt β-strand conformation.

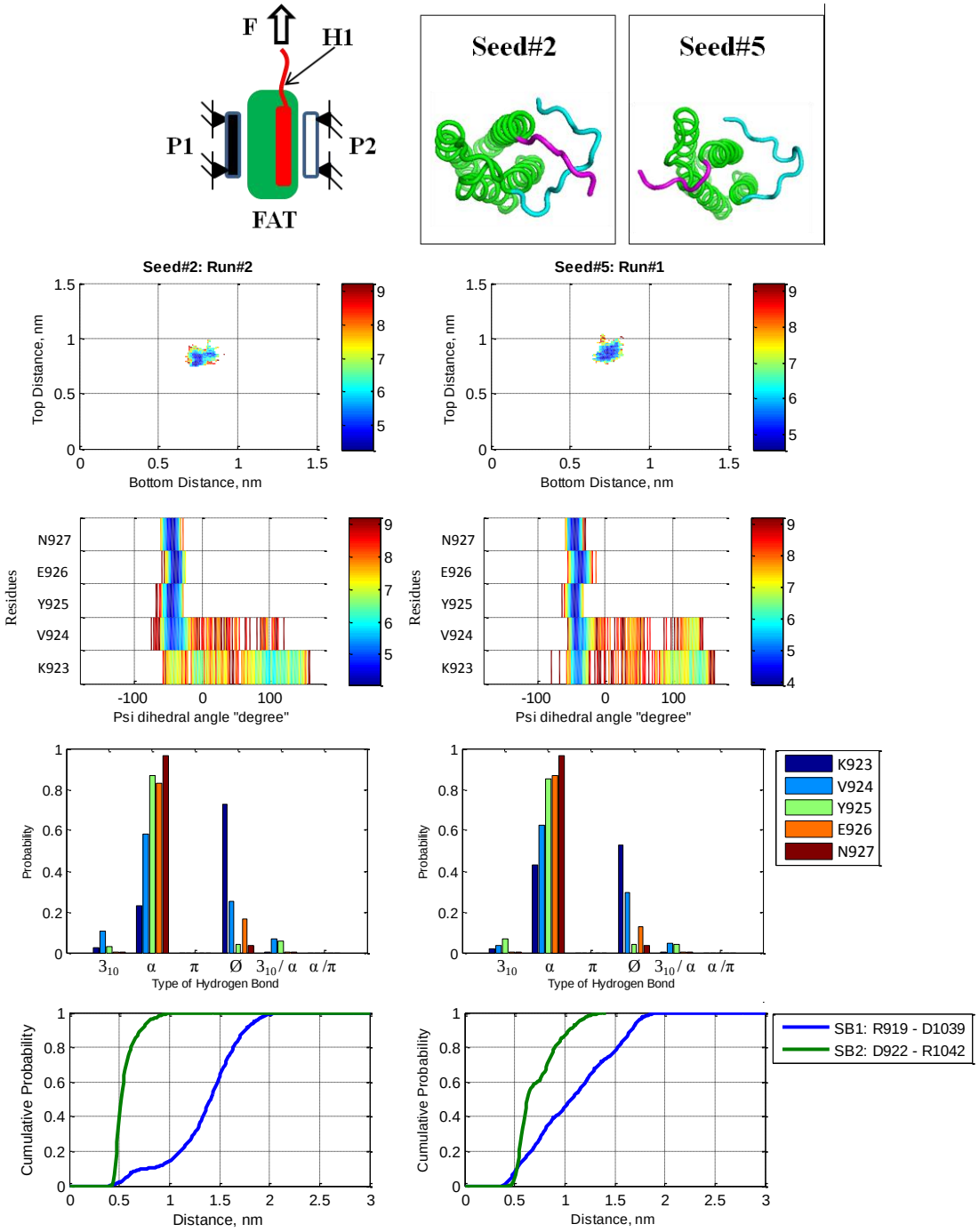


Figure 4-24: Four different matrices are shown for H1 atypical behavior; H1 position, dihedral angle ψ, hydrogen bond state and the salt bridge state. (Table 3-1, AX.WT.P1P2).

Figure 4-25 shows that the structure of the region flanking Y925 in its final state, as well as the probability of the number of interactions formed between the H1/H4 tail. The atypical behaviors of H1/H4 tail are different: one forms β-sheet via number of hydrogen bonds, while in the second, H1/H4 tail are separate. Even when H1/H4 tail share the applied load via forming β-sheet, it does not persist the unfolding of H1. This suggests that the interactions formed between H1/H4 tail might not have a significant effect on holding H1 to the bundle.

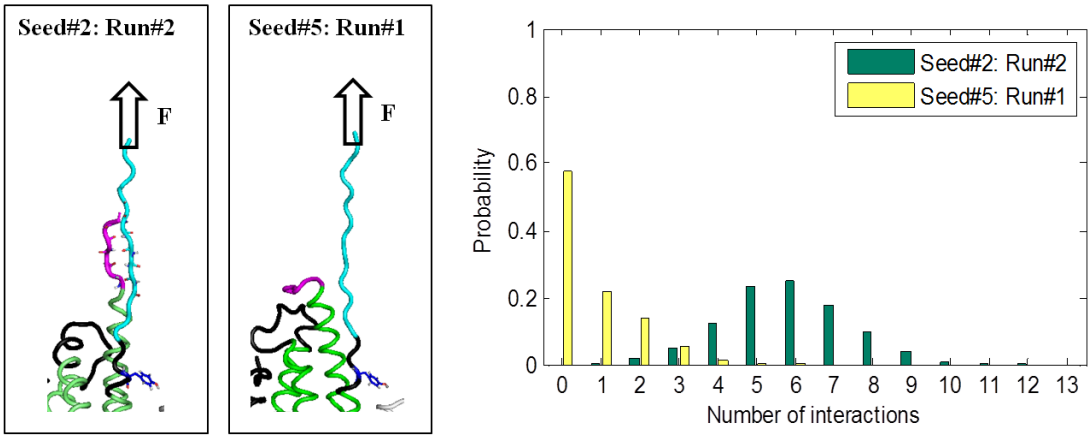


Figure 4-25: Two types of figure are shown for H1 atypical behavior; final state of the structure of the region flanking Y925, and number electrostatic interactions formed between H1/H4 tail. (Table 3-1, AX.WT.P1P2).

4.2.1.3 Axial Load Scenario Result Summary

For axial load scenario, a total of 200 ns simulation time was run. All simulations starts with different initial conditions (seeds, equilibration process and initial velocities). In general, none of these simulations shows that H1 comes out of the bundle. Also, there is a low propensity of the second residue (V924, besides K923) to unfold while all other residues are stable in a helical form. The two salt bridges are broken more often. H1/H4 tail prefer to interact with each other. In more than 80% of the simulations ran, the H1/H4 tail stay entangled via hydrogen and/or electrostatic interactions.

In some simulations, the salt bridges are broken and H1/H4 tail are separate, however, H1 is attached to the bundle. It has been suggested that in addition to the salt bridges, hydrophobic interactions (between highly hydrophobic residues, e.g., Val, Leu, and Ile) between H1 and the bundle create an energy barrier preventing H1 from leaving the bundle (Figure 4-26). They could be important in holding H1 to the bundle.

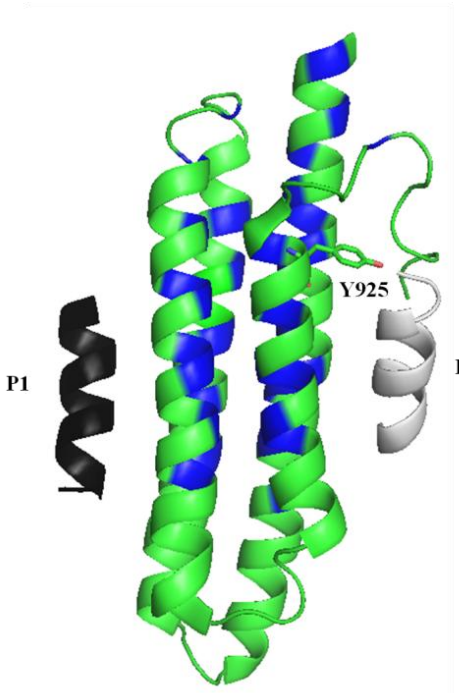


Figure 4-26: Highly hydrophobic resides between H1 and the bundle. The blue colored residues are either Val, Leu, or Ile. These residues create the hydrophobic core that may be responsible for holding H1 to the bundle.

Under 100 pN axial load applied to N-terminus to H1 tail, H1 does not appear to have a propensity to leave the bundle. The region flanking Y925 prefers to stay in a helical form. As discussed before, for Y925 phosphorylation, H1 has to leave the bundle and adopt β-strand conformation. So, it seems that the axial load scenario does not appear to have the capacity to promote the required structural changes for making Y925 accessible for phosphorylation.

Table 4-3: Final state of the structure of the region flanking Y925 for H1 typical and atypical behaviors under constant force applied axially to the N-terminus of H1 tail. (Table 3-1, AX.WT.P1P2).

	H1 Position		H1 Unfolding			H1/H4 Tail Interactions				H2-H3 Structure	
	In	Out	F	SUF	UN	β, EX	β, NEX	τ	S	F23	U23
Probability %	10/10	0/10	8/10	2/10	0/10	1/10	4/10	2/8	3/10	8/10	2/10

4.2.2 PERPENDICULAR LOAD SCENARIO RESULTS

Six different initial structures (Seeds, Figure 3-12) were chosen based on the behavior of H1/H4 tail, their relative position to each other, as well as how many interactions they have (Figure 3-11). Each seed was run twice, with different initial velocities (Table 3-1, PR.WT.P1). A 100 pN constant force is applied to the N-terminus of H1 tail in a direction perpendicular to the H1 axis and P1 was constrained. The results of the perpendicular load simulation show two types of H1 behavior: typical and atypical (Table 4-4).

Table 4-4: H1 typical and atypical behaviors under perpendicular load, applied to the N-terminus of H1 tail and P1 constrained. Nine out of twelve simulations have typical behavior, while three have atypical behavior. (Table 3-1, PR.WT. P1P2).

Initial Structures		H1 Behavior Type		H1 Behavior Description	
		Typical	Atypical	H1 Position	H1 Unfolding
Seed#1	Run#1	-	Yes	Out of the bundle	In a β-strand conformation
	Run#2	Yes	-	In the bundle	In a helical form
Seed#2	Run#1	-	Yes	In the bundle	In a β-strand conformation
	Run#2	Yes	-	In the bundle	In a helical form
Seed#3	Run#1	Yes	-	In the bundle	In a helical form
	Run#2	Yes	-	In the bundle	In a helical form
Seed#4	Run#1	Yes	-	In the bundle	In a helical form
	Run#2	Yes	-	In the bundle	In a helical form
Seed#5	Run#1	Yes	-	In the bundle	In a helical form
	Run#2	Yes	-	In the bundle	In a helical form
Seed#6	Run#1	-	Yes	In the bundle	The first two residues, K923 and V924, of H1 unfold.
	Run#2	Yes	-	In the bundle	In a helical form

4.2.2.1 H1 Typical Behavior

Nine simulations out of twelve have nominally the same H1 behavior (Table 4-4). These nine simulations started with different initial conditions (seeds and initial

velocities). Regardless of the differences in their initial conditions, the behavior of H1 is very similar. The typical behavior of H1 is similar to its behavior under equilibrium.

4.2.2.1.1 H1 Position

Figure 4-27 shows the blue-colored regions (minima) of the H1 position have small distribution. For all different initial conditions applied, the relative position of H1 to the bundle is very stable, which means H1 does not appear to have a propensity to leave the bundle. As discussed before, electrostatic and hydrophobic interactions between H1 (residues 917-922) and H4 present an energy barrier keeping H1 attached to the bundle. For these simulations, 100 pN constant load applied does not appear to have the ability to overcome this energy barrier. FAT domain tends to move as a rigid body and the 100 pN perpendicular load does not have the capacity to open the FAT domain out.

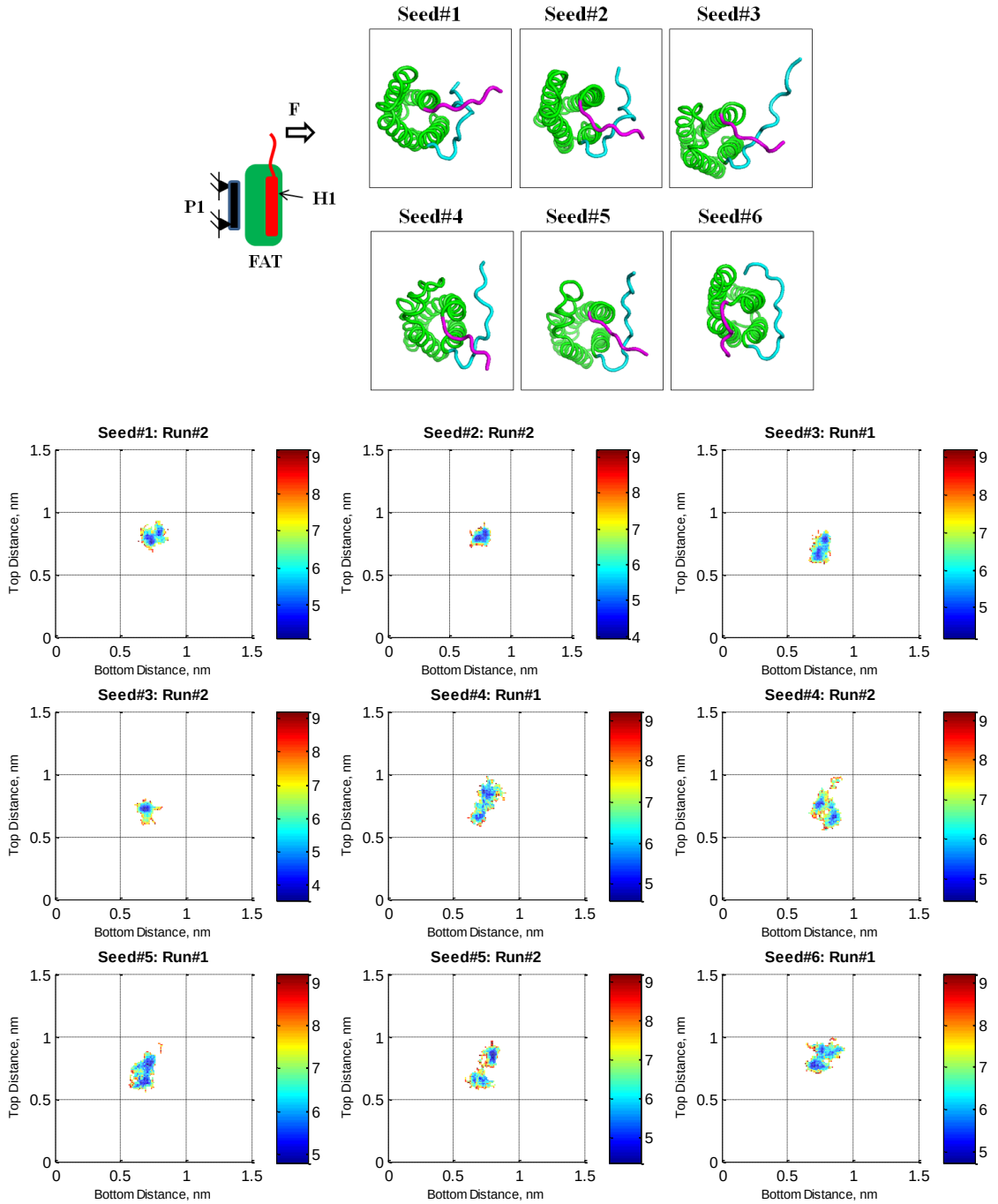


Figure 4-27: Energy landscape of H1 position represented by d_{top} and d_{bottom} in the absence of P2. For typical behavior, H1 position has a small distribution (minima) which means H1 does not appear to have the propensity to leave the bundle under constant force applied to the N-terminus of H1 tail perpendicular to the P1 axis. Each plot represents a simulation time of 20 ns. (Table 3-1, PR.WT.P1).

4.2.2.1.2 H1 Unfolding

4.2.2.1.2.1 Backbone Dihedral Angle ψ

Figure 4-28 shows that except residue K923, the ψ angles of the other top four residues of the H1's N-terminal (V924, Y925, E926, and N927) have a small distribution (the mean value is ~ -50^0 degree). This means they are folded in a helical form. However, the first residue at the N-terminus of H1 (K923) is expected, as discussed before, to have a greater flexibility, since it connects with H1 tail (i.e., H1 tail is free to move). The flexibility of K923 does not affect the stability of the other residues flanking Y925. This figure also shows that in Seed#4 Run#1, the residue V926 is the most damaged one. However, Figure 4-29 shows that the residues V926 refolded back after the unfolding and they do not stay unfolded.

For all simulations had been discussed, the region flanking Y925 does not appear to have the propensity to adopt β-strand conformation. Even residue K923 has a propensity to unfold, all other residues are stable and not affected by its flexibility. This means H1 has a high resistance to any structural rearrangements needed for making Y925 accessible for phosphorylation.

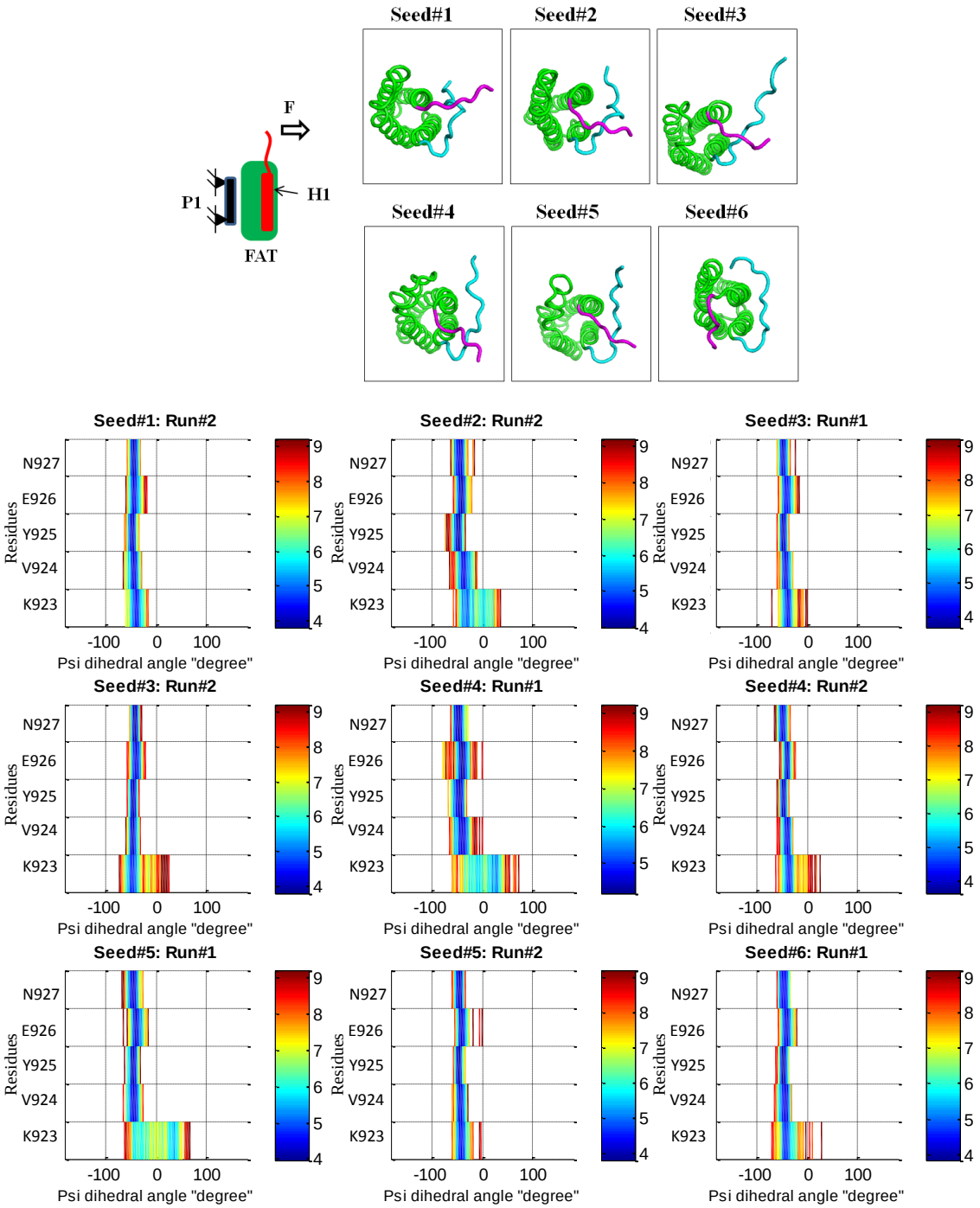


Figure 4-28: Energy landscape of the dihedral angle ψ of the five N-terminal residues of H1 (K923, V924, Y925, E926, and N927) in the presence or the absence of P2 for H1 typical behavior. Except N923 that have greater flexibility, since it connects with the floppy tail (H1 tail), ψ angle of other residues have a small distribution (minima). This means H1 does not appear to have the propensity to adopt β-strand conformation under constant force applied to the N-terminus of H1 tail perpendicular to the P1 axis. Each plot represents a simulation time of 20 ns. (Table 3-1, PR.WT.P1).

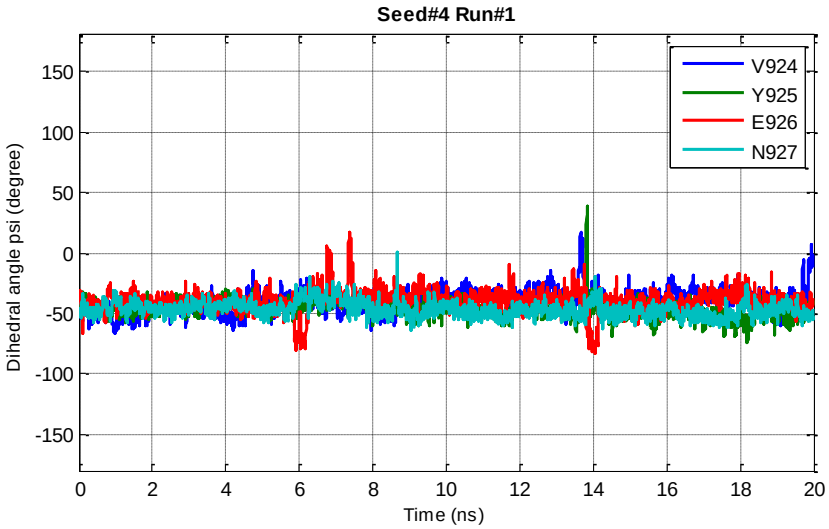


Figure 4-29: Dihedral angle ψ of the four N-terminal residues of H1 (V924, Y925, E926 and N927) versus time in absence of P2. For Seed#4 Run#1, the ψ angle of V924 and E926 shows that they refold after unfolding (Table 3-1, PR.WT.P1).

4.2.2.1.2.2 Hydrogen Donor-Accepter Pairs

Figure 4-30 shows the probability of different hydrogen bond types formed by the first five residues at the N-terminal of H1 (K923, V924, Y925, E926, and N927). Most the time, they form an α-helix hydrogen bond type for any different initial conditions applied. The π and 3_{10}-helix hydrogen bond type formed very rarely. The hydrogen bond of K923 is broken about ~ 50% of the time. However, the hydrogen bonds of other four residues are broken about 3 ~ 15% of the time. The residue K923 is expected to have more broken hydrogen bond since it connects to the H1 tail.

Hydrogen donor-acceptor pairs metric is useful in examining the propagation of the unfolding, if any. Based on what Figure 4-30 shows, the unfolding of K923, in most of the simulations, does not propagate into the other four residues where they are stable.

Neither thermal fluctuation nor 100 pN load appear to excite the region flanking Y925 and promote the needed conformational rearrangements for the phosphorylation.

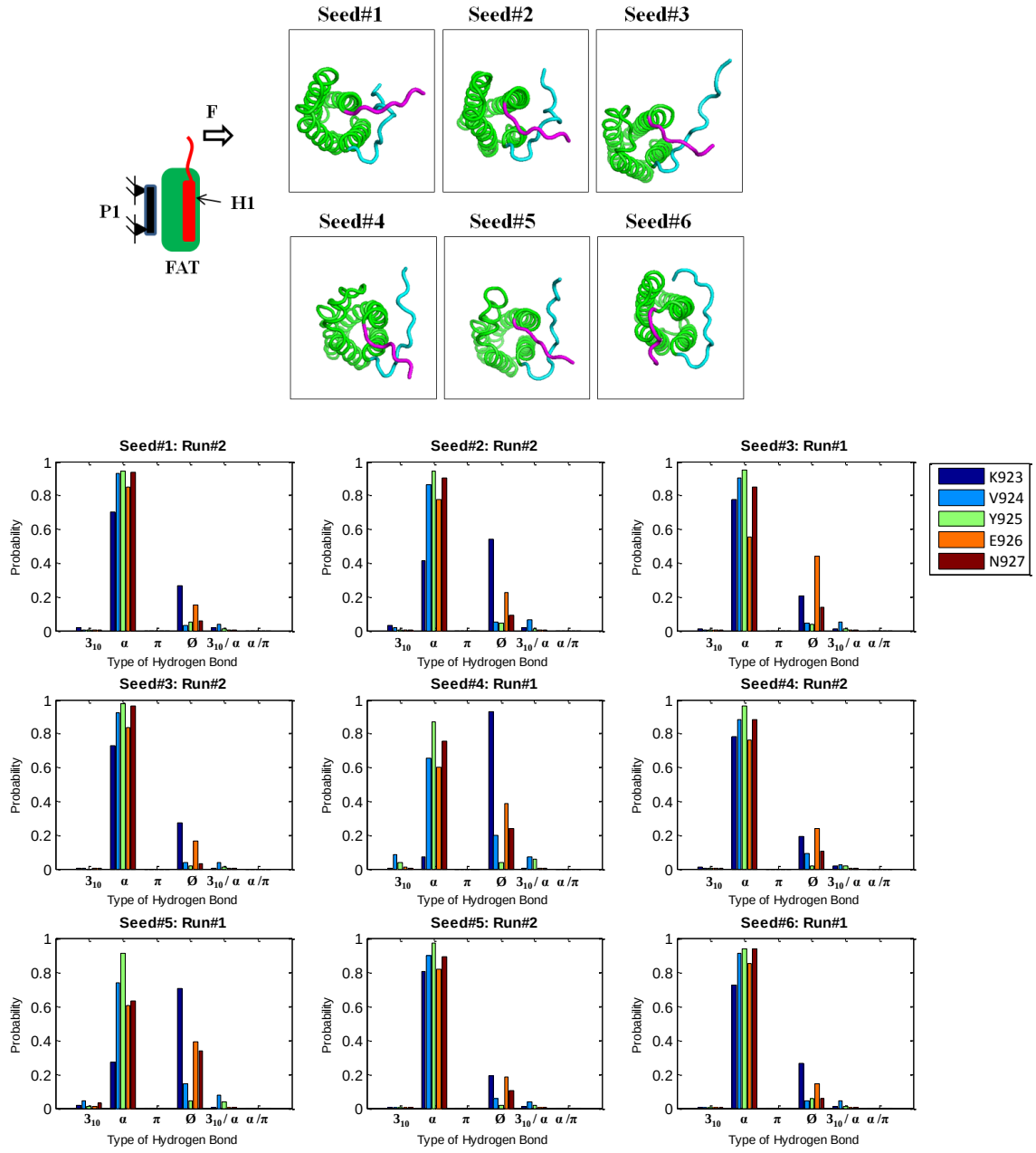


Figure 4-30: Hydrogen bonds types formed in the absence of P2. For H1 typical behavior, H1 primarily forms an α-helix. Each plot represents a simulation time of 20 ns. (Table 3-1, PR.WT.P1).

4.2.2.1.3 Salt Bridges between H1 Tail and H4

Figure 4-31 shows the wide distribution of distances between residues that formed the two salt bridges (SB1: R919-D1039, SB2: D922–R1042). This wide distribution of the distance means they are broken most the time. The first salt bridge (SB1) has a wider distribution than the second one (SB2), which is because of the load applied to H1 tail. The H1 tail is pulled in a direction that breaks the first salt bridge more often and pulls the residue, N916, that sometime interacts with R1042, making the second salt bridge more stable. (Figure 4-31). The applied load makes the first salt bridge weaker and the second salt bridge stronger.

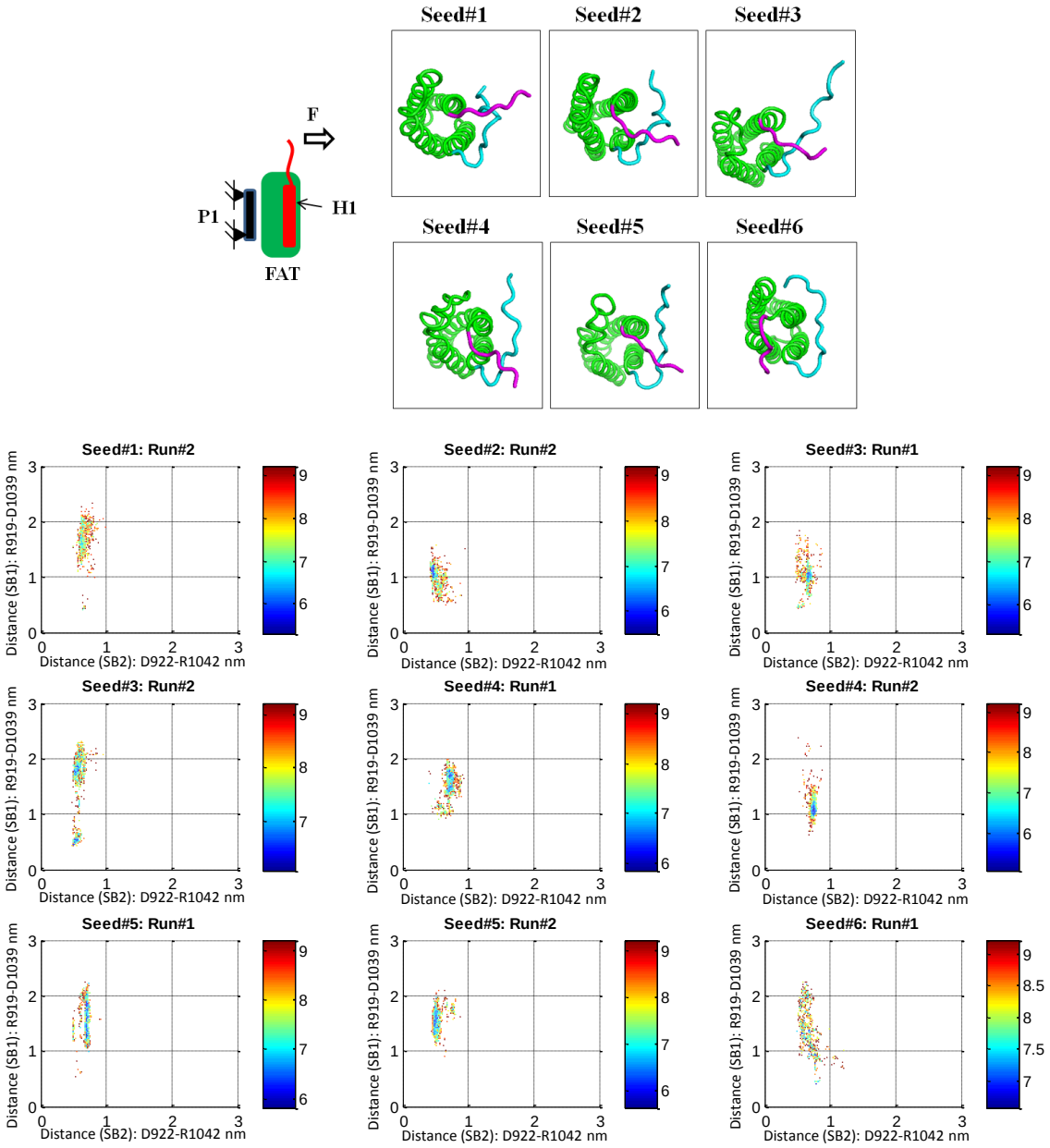


Figure 4-31: Energy landscape of the H1/H4 salt bridge distances represented by SB1 (R919–D1039) and SB2 (D922–R1042). SB1 and SB2 have a wide distribution which means they are broken. This suggests that they are not primarily responsible for keeping H1 folded within the bundle. Each plot represents a simulation time of 20 ns. (Table 3-1, PR.WT.P1).

As seen in Figure 4-32, if the salt bridge distance must be less than 0.5 nm, then the first salt bridge, SB1: R919–D1039, is broken most the time, whereas the second one, SB2: D922–R1042, persists 30% of the time. Under the influence of the perpendicular load, the relative position of H1 tail to the bundle increases, which makes the first salt bridge break more of time and point the residue, D922, to R1042 closer than N916 (Figure 4-20).

However, as discussed before, these salt bridges have been suggested, among other factors, to be responsible of maintaining relative position of H1 with the bundle. This result suggests that it does not appear that these salt bridges have a significant role in keeping H1 attached to the bundle. In addition, salt bridge metric suggests that the strength of the interactions between the residues are affected by the applied load which is consistent with the axial load results.

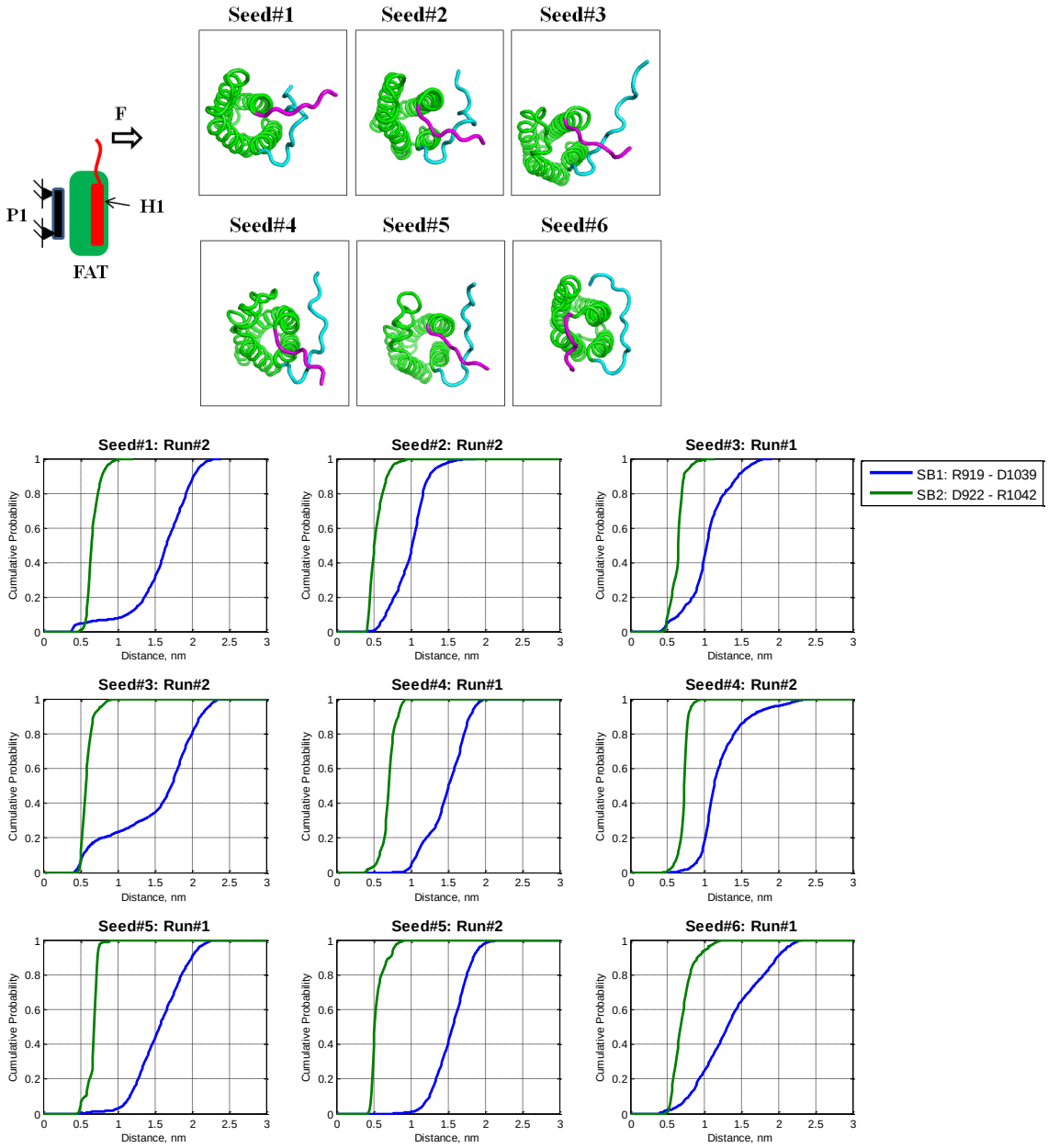


Figure 4-32: Cumulative probability of the two salt bridges represented for two distances, SB1 (R919–D1039) and SB2 (D922–R1042). If the salt bridge distance has to be less than 0.5 nm, it means they are broken ~70%. This suggests that they are not primarily responsible for keeping H1 folded within the bundle. Each plot represents a simulation time of 20 ns. (Table 3-1, PR.WT.P1).

4.2.2.1.4 H1/H4 Tail Interaction

Figure 4-33 shows how many interactions formed between the H1/H4 tail. The number of H1/H4 tail interactions is widely distributed, in which Seed#3 Run#2 and Seed#6 Run#1 are different than the others. In these two simulations, H1/H4 tail have almost no interactions, where their initial structures are different in terms of H1/H4 tail behavior. In Seed#3, they interact with each other, while in Seed#6, they are separate. In second runs of Seed#1 and Seed#5, H1/H4 tail have 1~3 electrostatic interactions in between while in other five simulations, H1/H4 tail are entangled through 4 ~7 electrostatic interactions. In Seed#3, Run#2 and Seed#6, Run#1, even the two salt bridges are broken and the H1/H4 tail are separate, H1 is strongly attached to the bundle in a helical form. This suggests that there are another factors that holding H1 to the bundle which is hydrophobic interactions that has been discussed § 4.2.1.3 Axial Load Result Summary.

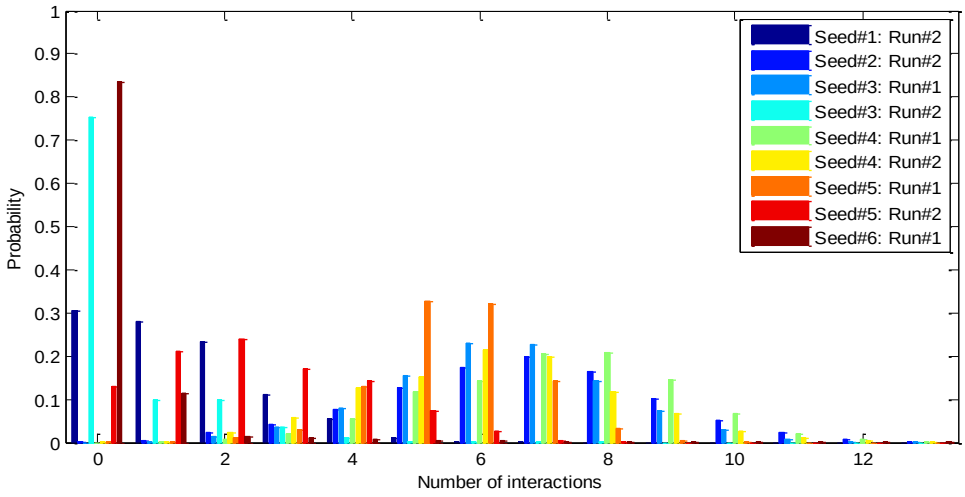


Figure 4-33: Number electrostatic interactions formed between H1/H4 tail. The interactions between H1/H4 have a wide distribution which means H1/H4 tail prefer to entangled. Each bar represents a simulation time of 20 ns. (Table 3-1, PR.WT.P1).

4.2.2.1.5 FAT Structure in its Final States

Table 4-5 shows show the FAT structure's final states in terms of H position, H1 unfolding, H1/H4 tail interactions and H2-H3 structure. For 100% of the nine simulations, H1 stays folded in the bundle. In more than 50% of the simulations, H1/H4 tail form β-sheet via a number of hydrogen bonds. In about 25%, they are entangled via number of electrostatic interactions. This suggests that H1/H4 tail prefer to interact with each other more often. In two simulations (Seed#3, Run#2 and Seed#6, Run#1), H1/H4 tail are mostly separate. (H1/H4 tail interactions are listed in (Appendix D). In these two simulations, H1 stays folded in the bundle, which suggests that H1/H4 tail does not appear to be the key regulator of resisting H1 unfolding or keeping H1 attached to the bundle.

Table 4-5: Final state of the structure of the region flanking Y925 for H1 typical behavior under constant force applied perpendicularly to the N-terminus of H1 tail. (Table 3-1, PR.WT.P1).

	H1 Position		H1 Unfolding			H1/H4 Tail Interactions				H2-H3 Structure	
	In	Out	F	SUF	UN	β, EX	β, NEX	τ	S	F23	U23
Probability %	9/9	0/9	9/9	0/9	0/9	0/9	5/9	2/8	2/9	7/9	2/9

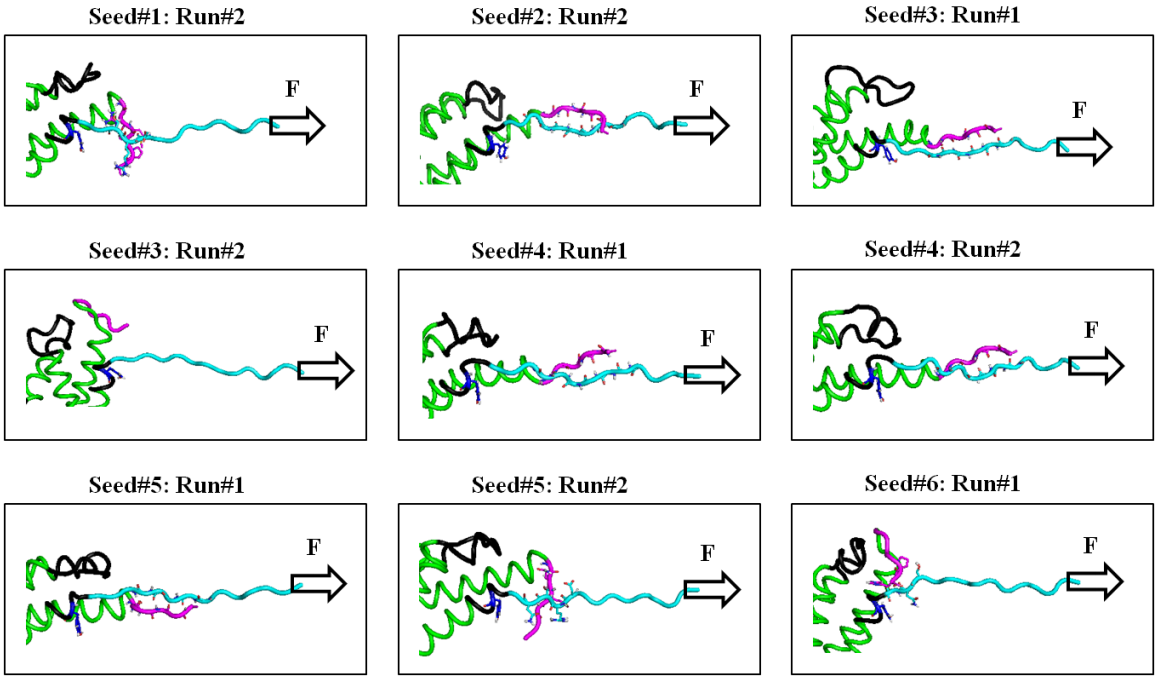


Figure 4-34: Final state of the structure of the region flanking Y925 for H1 typical behavior under constant force applied perpendicularly to the N-terminus of H1 tail. (Table 3-1, PR.WT.P1).

4.2.2.2 H1 Atypical Behavior

Figure 4-35 shows four different metrics: H1 position, dihedral angle ψ, hydrogen state and salt bridge state. For two simulations (Seed#2, Run#1 and Seed#2, Run#1), the relative position of H1 has a small distribution (blue-colored region) which means H1 is attached to the bundle. However, in Seed#1, Run#1, the top distance between H1 and neighbor helices has a wide distribution. For this simulation, Figure 4-36 shows that the top distance between H1 and neighbor helices increases rapidly which means H1 come out of the bundle.

Also, in Seed#1, Run#1 and Seed#2, Run#1, the ψ angle of the top five residues unfolded and reach 170^0, which means they adopt β-strand conformation. In Seed#6 Run#1, only the top two residues of H1 (K923 and V924) have a propensity to unfold while the others remain folded.

In Seed#1, Run#1 and Seed#2, Run#1, the hydrogen bonds of the top five residues of H1 are mostly broken. Whereas, in Seed#6, Run#1, the unfolding of the first two residues of H1 (K923, V924) does not propagate into the other residues. In addition, for all the three simulations, the salt bridges are broken more often.

In only one simulation, atypical behavior of H1 achieved the required structural changes needed for Y925 phosphorylation, where H1 leaves the bundle and adopt β-strand conformation.

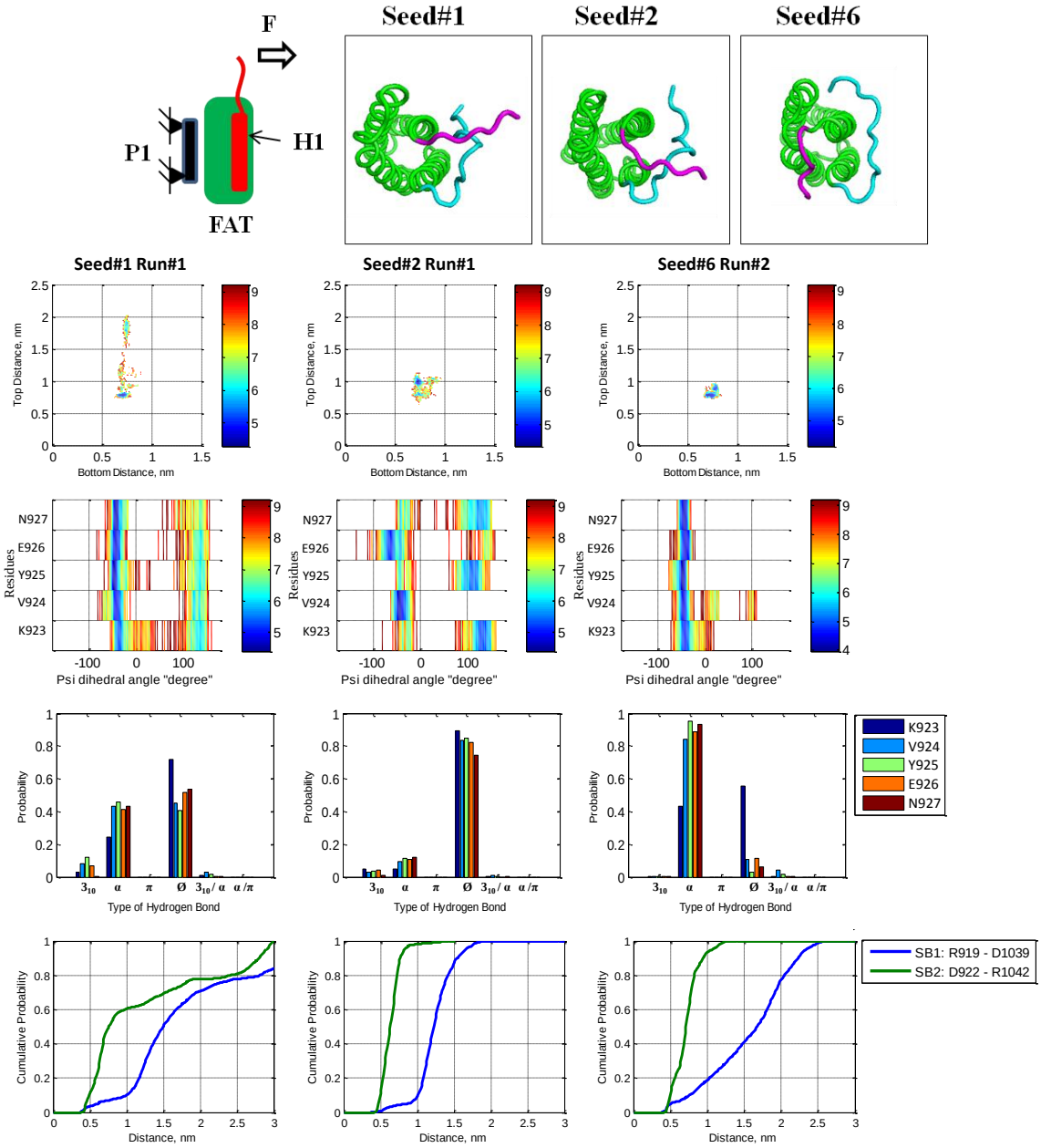


Figure 4-35: Four different matrices are shown for H1 atypical behavior; H1 position, dihedral angle ψ, hydrogen bond state and the salt bridge state. (Table 3-1, PR.WT.P1).

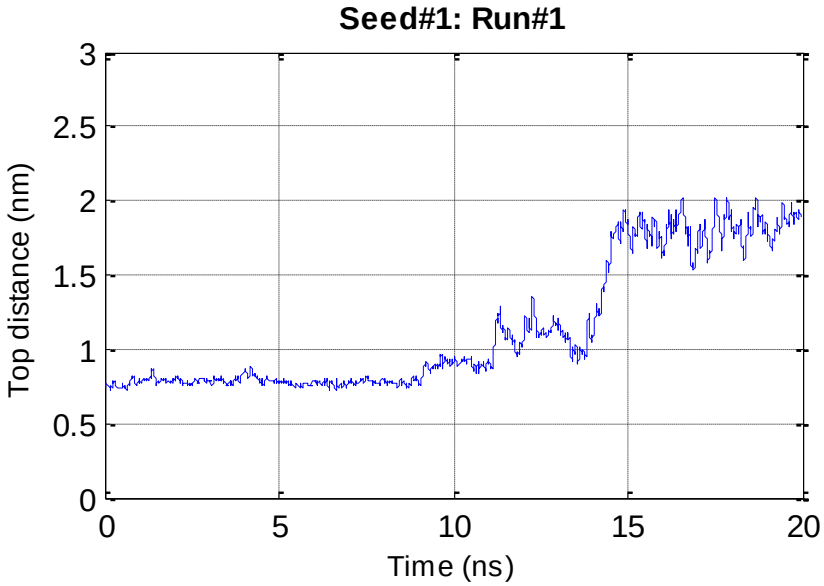


Figure 4-36: H1 position represented by d_{top} versus time for H1 atypical behavior. The d_{top} increases rapidly as H1 leaves the bundle.

Figure 4-37 shows that the structure of the region flanking Y925 in its final state, as well as the probability of the number of interactions formed between the H1/H4 tail. The atypical behaviors of H1/H4 tail are different: in one simulation, they form β-sheet via number of hydrogen bonds (Seed#2, Run#1), while in two other simulations (Seed#1, Run#1 and Seed#6, Run#2), the H1/H4 tail are separate.

Even when H1/H4 tail share the applied load via forming β-sheet, H1 does not come out of the bundle. Moreover, H1 stays in the bundle while H1/H4 tail are separate. This suggests that the interactions formed between H1/H4 tail might not have a significant effect on holding H1 to the bundle.

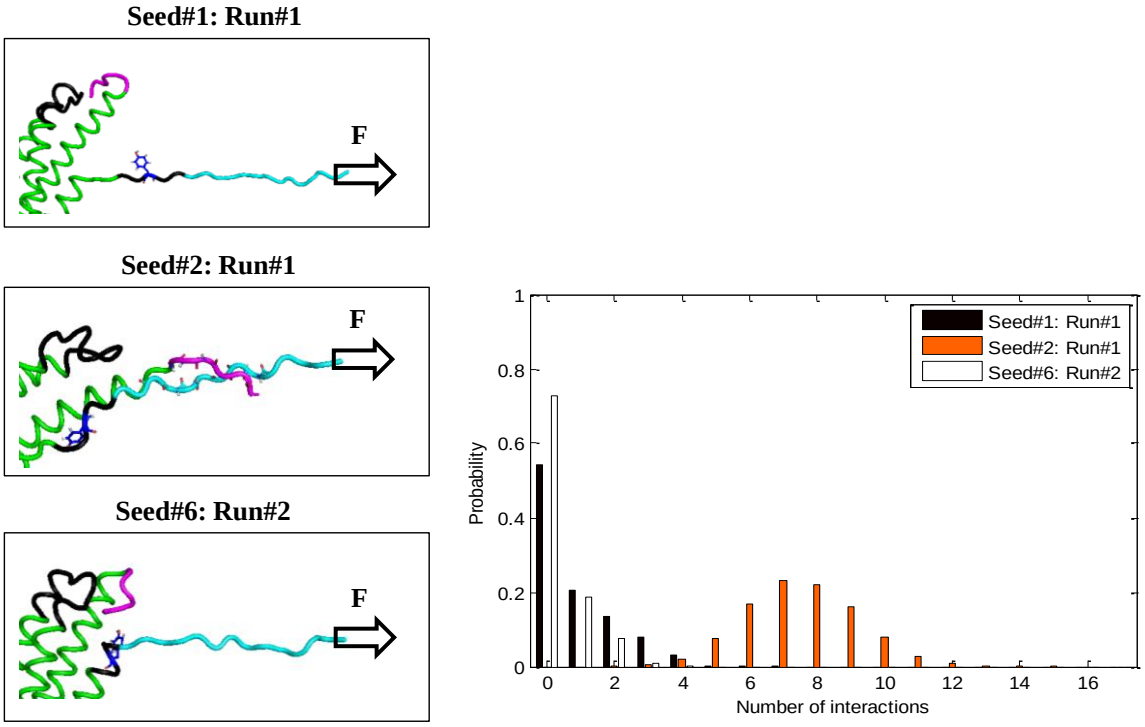


Figure 4-37: Two types of figure are shown for H1 atypical behavior; final state of the structure of the region flanking Y925, and number electrostatic interactions formed between H1/H4 tail. (Table 3-1, PR.WT.P1).

Since Seed#1 shows one simulation that FAT undergoes the required structural rearrangement needed for Y925 phosphorylation, it is important to run more simulations for this seed with different initial velocities. The goal is to examine the repeatability of the atypical type of behavior in which H1 is out of the bundle and it adopts a β-strand conformation.

4.2.2.3 Repeatability of H1 Atypical Behavior

Under mechanical load applied perpendicular to the N-terminus of H1 tail, nine more simulations of Seed#1 were run to examine the repeatability of the atypical

behavior of H1, where the region flanking Y925 adopts β-strand and comes out of the bundle.

4.2.2.3.1 H1 Position

As seen in Figure 4-38, the blue-colored regions (minima) of the H1 position have small distribution. For all different initial velocities applied, the relative position of H1 to the bundle is very stable. This means H1 prefers to be within the bundle and atypical behavior, where H1 comes out of the bundle, is not repeatable. This emphasizes how strong the energy barrier that keeps H1 within the bundle.

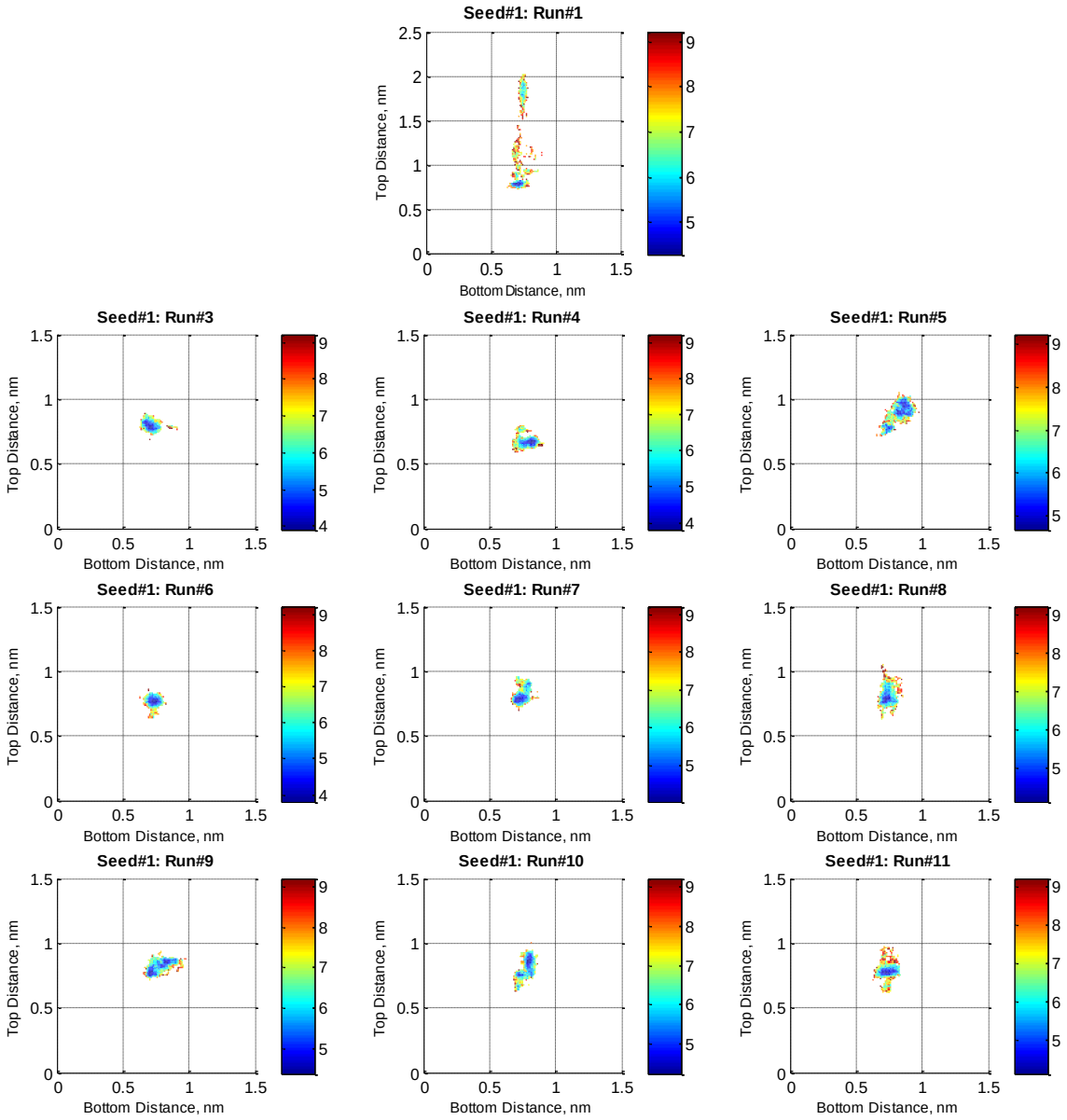


Figure 4-38: Energy landscape of H1 position represented by d_{top} and d_{bottom}. Looking to the repeatibility of H1 atypical behavior found in Seed#1 Run#1, H1 position has a small distribution (minima) which means H1 does not appear to have the propensity to leave the bundle under constant force applied to the N-terminus of H1 tail perpendicular to the P1 axis. The H1 atypical behavior is not repeatable in terms of H1 position. Each plot represents a simulation time of 20 ns. (Table 3-1, PR.WT.P1).

4.2.2.3.2 H1 Unfolding

4.2.2.3.2.1 Backbone Dihedral Angle ψ

As in Figure 4-39, the ψ angle of the top five residues (except K923) for six different simulations, has small distribution which means they have the capacity to keep their helical conformations. In Seed#1, Run8, only the first two residues have the propensity to unfold, while other residues are very stable. In Seed#1, Run#10, only three residues out of five have the propensity to unfold. In general, it appears that the atypical behavior of H1, where the region flanking 925 adopts β-strand conformation, is not repeatable.

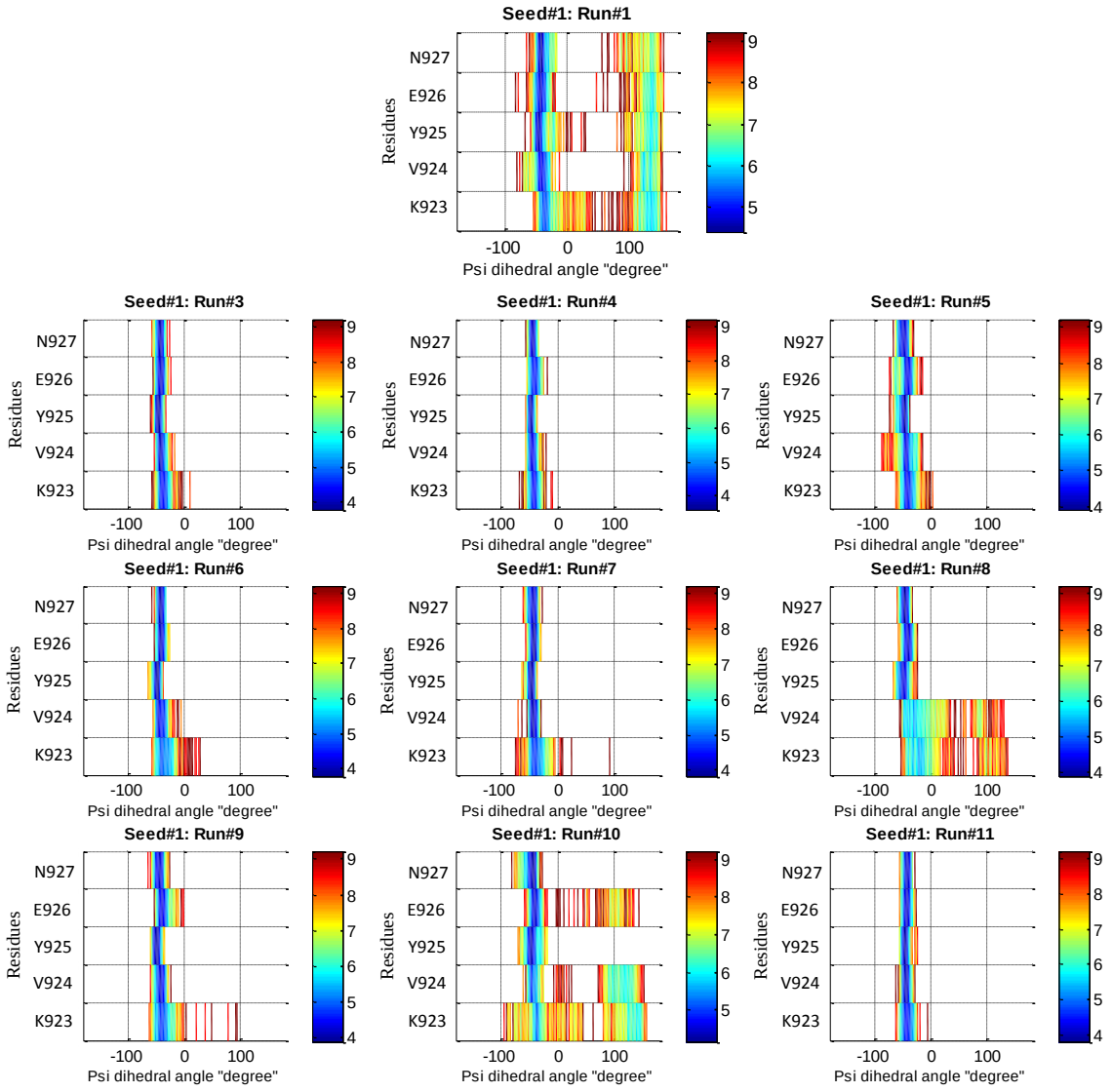


Figure 4-39: Energy landscape of the dihedral angle ψ of the five N-terminal residues of H1 (K923, V924, Y925, E926, and N927) in the presence or the absence of P2 for H1 atypical behavior repeatability. Except Seed#1, Run#8 and Seed#1, Run#10, ψ angle have a small distribution (minima), which means H1 atypical behavior is not repeatable in terms of adopting a β-strand. For Seed#1, Run#8 and Seed#1, Run#10, some residues have a tendency to unfold (Seed#1, Run#8: V924, Seed#1, Run#10: V924 and E926). (Table 3-1, PR.WT.P1).

4.2.2.3.2.2 Hydrogen Donor-Accepter Pairs

Figure 4-43 shows that the only simulation that has similarity with atypical behavior is Seed#1, Run#10, in which the hydrogen bonds of the first five residues are broken are mostly broken. Otherwise, in the other simulations the first five residues of H1 form α-helix hydrogen bond type. This supports the previous results that suggest the atypical behavior is not repeatable.

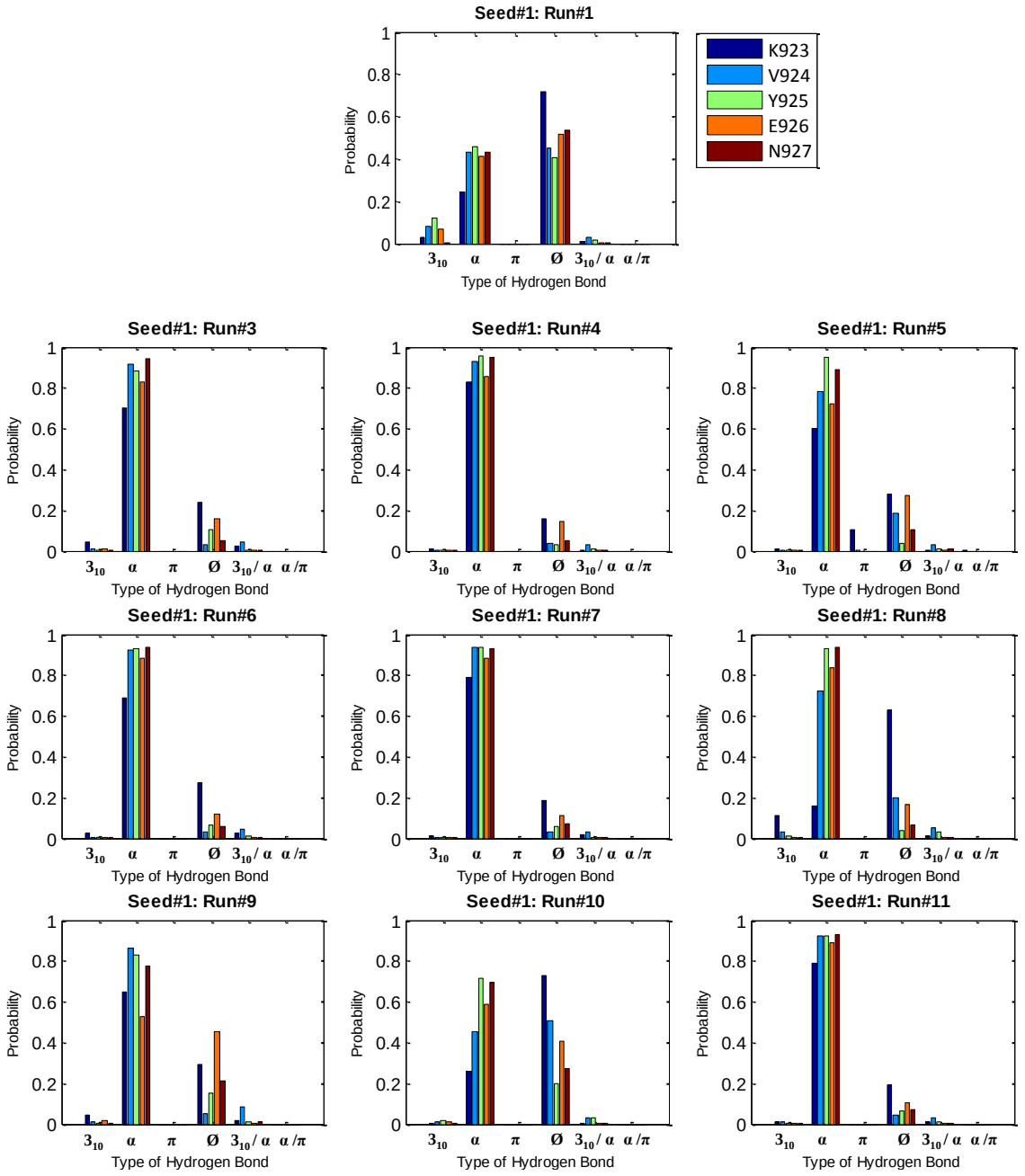


Figure 4-40: Hydrogen bonds types formed in the absence of P2. For the repeatability of H1 atypical behavior and except Seed#1, Run#10, H1 primarily forms an α-helix. In general, the H1 atypical behavior is not repeatable in terms of the hydrogen broken. Each plot represents a simulation time of 20 ns. (Table 3-1, PR.WT.P1).

4.2.2.3.3 Salt Bridges between H1 Tail and H4

As seen in Figure 4-41 and Figure 4-42, the wide distribution of the two salt bridge distances suggests that they are broken most the time. This is consistent with the previous results that these salt bridges are not the key regulator of holding H1 to the bundle.

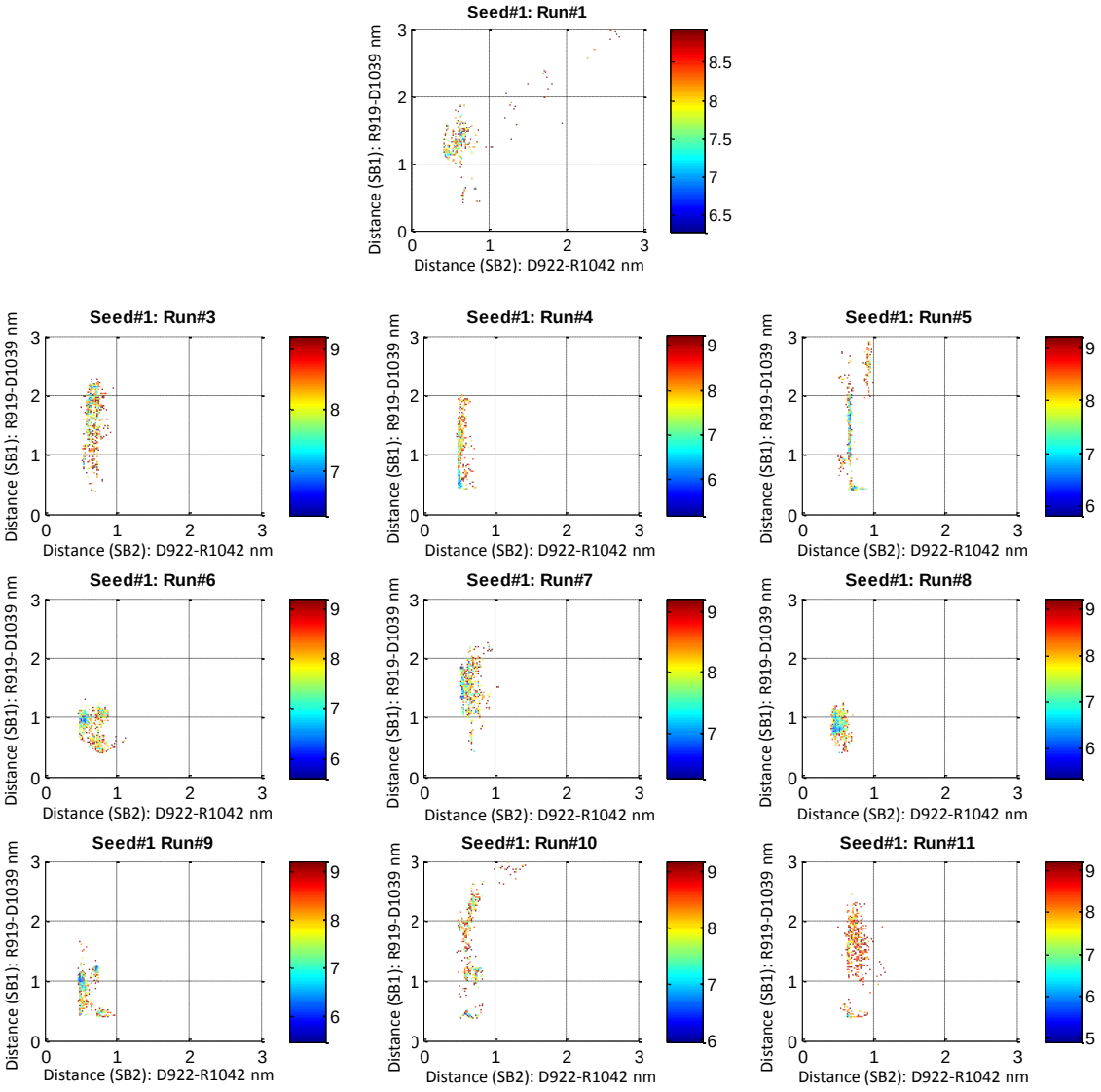


Figure 4-41: Energy landscape of the H1/H4 salt bridge distances represented by SB1 (R919–D1039) and SB2 (D922–R1042). SB1 and SB2 have a wide distribution which means they are broken. This suggests that they are not primarily responsible for keeping H1 folded within the bundle. Each plot represents a simulation time of 20 ns. (Table 3-1,PR.WT.P1).

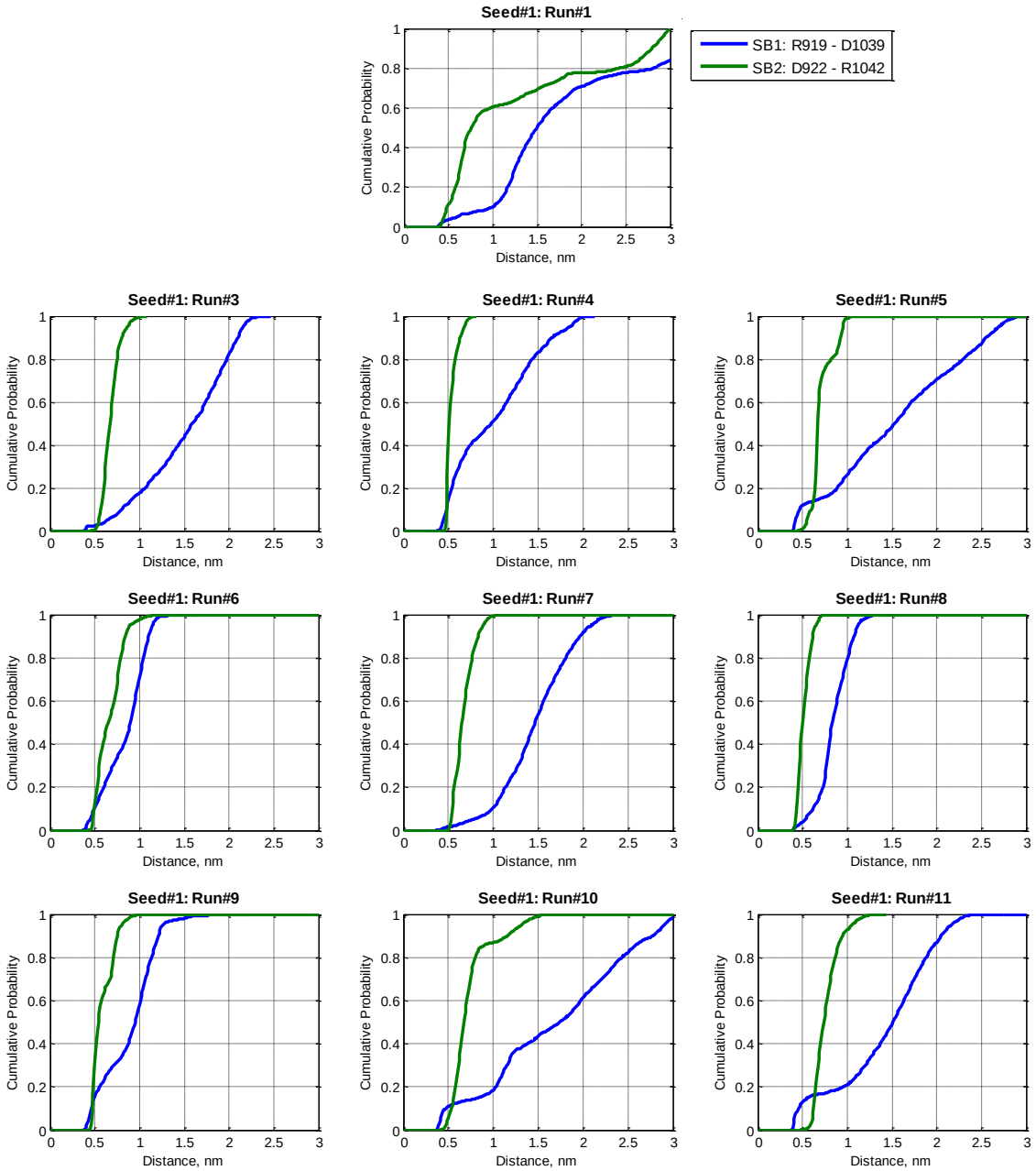


Figure 4-42: Cumulative probability of the two salt bridges represented for two distances SB1 (R919–D1039) and SB2 (D922–R1042). If the salt bridge distance has to be less than 0.5 nm, it means they are broken ~70%. This suggests that they are not primarily responsible for keeping H1 folded within the bundle. Each plot represents a simulation time of 20 ns. (Table 3-1, PR.WT.P1).

4.2.2.3.4 H1/H4 Tail Interaction

Figure 4-43 shows how many interactions formed between the H1/H4 tail. The number of H1/H4 tail interactions is widely distributed, which means H1/H4 tail prefers to be entangled through either hydrogen bonds or electrostatic interactions. In Seed#1, Run#11, even the two salt bridges are broken, the H1/H4 tail are separate, H1 is strongly attached to the bundle in a helical form. This suggests that they are another factors that holding H1 to the bundle. (discussed § 4.2.1.3 Axial Load Result Summary)

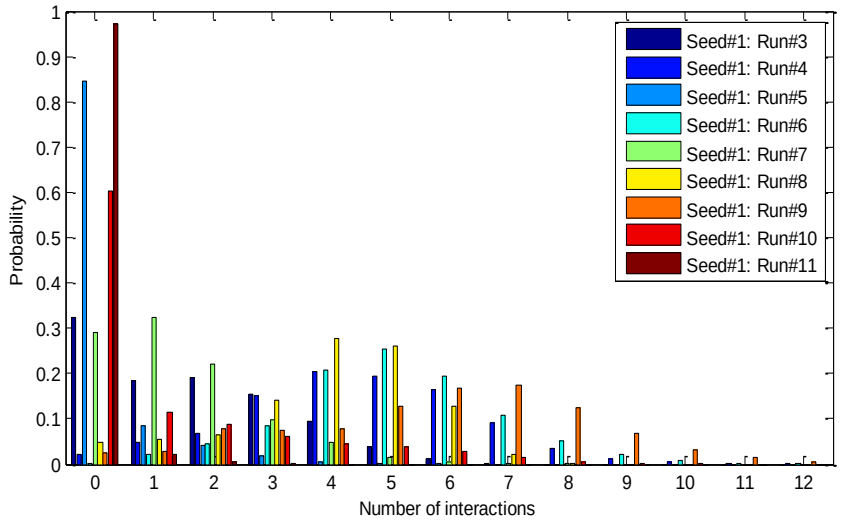


Figure 4-43: Number electrostatic interactions formed between H1/H4 tail. The interactions between H1/H4 have a wide distribution which means H1/H4 tail prefer to be entangled. Each bar represents a simulation time of 20 ns. (Table 3-1, PR.WT.P1).

4.2.2.3.5 FAT Structure in its Final States

Figure 4-44 show the FAT structure's final states in terms of H1 position, H1 unfolding, H1/H4 tail interactions and H2-H3 structure. For all nine simulations, H1 stays folded in the bundle. In 30% of the simulations, the H1/H4 tail form β-sheet via a number of hydrogen bonds. In about 20%, they are entangled via number of electrostatic

interactions. This suggests that H1/H4 tail prefer to interact with each other more often. In two simulations (Seed#1, Run#3 and Run#11), the H1/H4 tail are almost separate. (H1/H4 tail interactions are listed in (Appendix D). In these two simulations, H1 stays folded in the bundle, which suggests that H1/H4 tail does not appear to be the key regulator of resisting H1 unfolding or keeping H1 attached to the bundle. In Seed#1, Run#5, the FAT domain disassociates from the paxillin. This type of behavior raises the question of the loading capability of the FAT/paxillin complex. How much the maximum load can be hold by the paxillin needs more investigations.

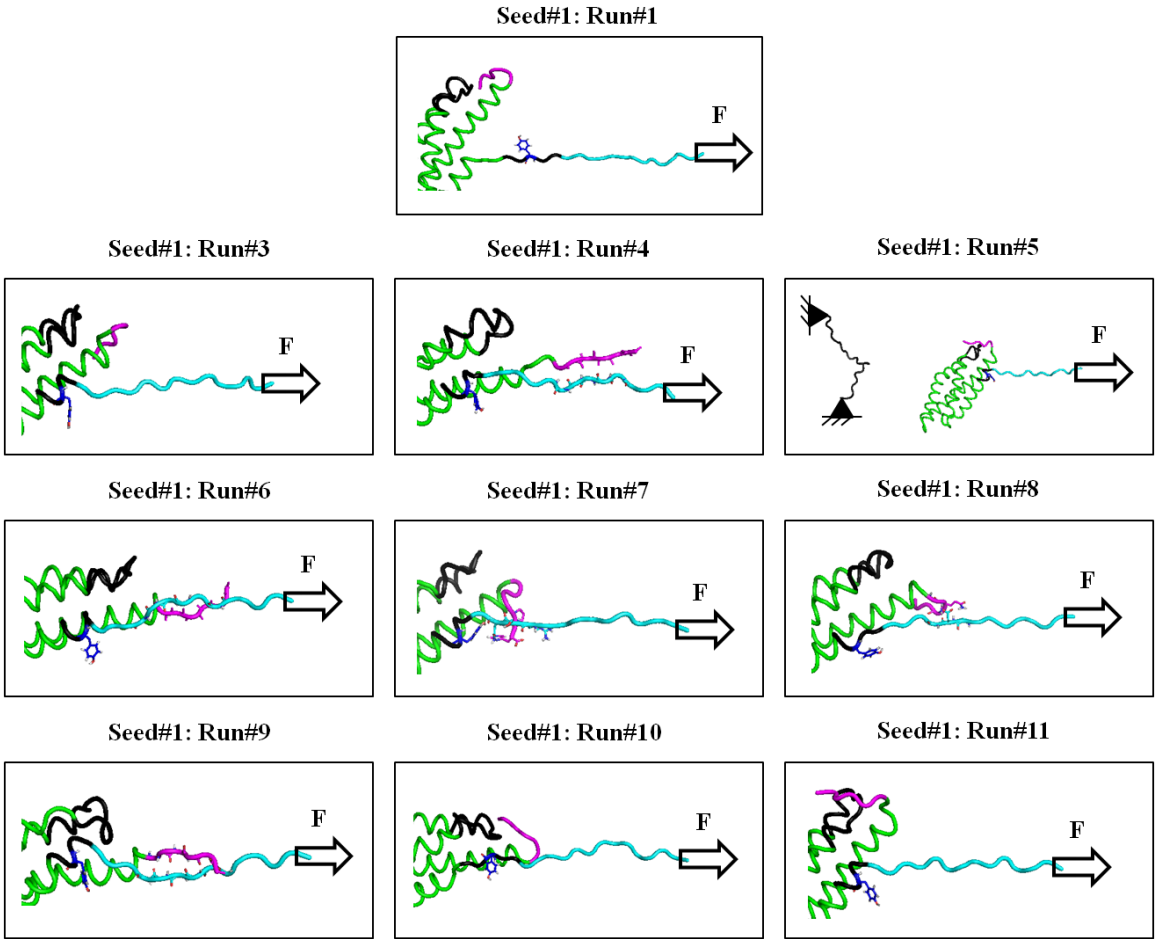


Figure 4-44: Final state of the structure of the region flanking Y925 under constant force applied perpendicularly to the N-terminus of H1 tail. (Table 3-1, PR.WT.P1).

4.2.2.4 Perpendicular Load Scenario Result Summary

For perpendicular load scenario, a total of 320 ns simulation time was run. All simulations starts with different initial conditions (seeds, equilibration process and initial velocities). In general, they show H1 has high propensity to be attached to the bundle. Also, H1 prefers to stay in a helical form. In most of the simulations, H1/H4 tail prefer to interact with each other. (See Table 4-6)

In only one simulation, H1 comes out of the bundle and the region flanking Y295 adopts a complete β-strand conformation. The same seed that shows this type of behavior, was run nine additional times with different initial velocities to examine the repeatability of this interesting type of behavior. However, none of the nine simulations shows the same behavior. This illustrates the low appearance of this type of behavior where H1 come out the bundle and the region flanking Y925 adopts β-strand conformation.

In one simulation, the FAT domain disassociates from the paxillin, which raises the question of the loading capability of the FAT/paxillin complex. It is important to examine how much load could paxillin holds.

Table 4-6: Final state of the structure of the region flanking Y925 for H1 typical and atypical behaviors under constant force applied perpendicularly to the N-terminus of H1 tail. (Table 3-1, PR.WT.P1).

	H1 Position		H1 Unfolding			H1/H4 Tail Interactions				H2-H3 Structure	
	In	Out	F	SUF	UN	β, EX	β, NEX	τ	S	F23	U23
Probability	20/21	1/21	16/21	2/21	3/21	1/21	8/21	4/21	8/21	17/21	4/21

Chapter 5. Conclusions

It has been reported that Y925 in the FAT domain is a critical phosphorylation site, key in cancer initiation and progression. In order for Y925 to be phosphorylated, it has been suggested that H1 has to come out of the bundle and the region flanking this tyrosine residue has to adopt β-strand conformation. What it takes the FAT domain to adopt the hypothesized structure, to engage the phosphorylation, remains unclear. So, it is very important to examine these hypotheses to have better understanding of FAT domain behavior which may contribute in anti-cancer therapy development. To accomplish this, Molecular Dynamics (MD) simulations and Constant Force Molecular Dynamics (CFMD) simulations were run. Two structures were used in the simulation: (i) the FAT/paxillin complex without H4 tail and P1/P2 unconstrained and (ii) the augmented FAT/paxillin complex with H4 tail and P1/P2 constrained. These two structures were used in different cases where the presence/absence of P1 and P2 was varied. All the simulations were run on a variety of initial conditions (different energy minimization and equilibration process, different initial velocities, different initial structures or "seeds"). The behavior of H1 that contains Y925 was examined using four different metrics: H1 position, H1 unfolding, salt bridge state, and H1/H4 tail interactions.

5.1 Under Equilibrium, Y925 Phosphorylation Conditions Not Met

Under thermal fluctuations only, H1 does not appear to have a proclivity to leave the bundle and/or adopt β-strand conformation. Both two FAT/paxillin structures were used in equilibrium simulation where the presence/absence of P1/P2 was varied. In addition, an isolated H1 helix and an isolated LD4 motif were simulated under

equilibrium conditions. The total equilibrium simulation time is 540 ns. Based on the equilibrium results, H1 is highly attached to the bundle and it does not appear to have a capacity to leave the bundle under only thermal fluctuation. Moreover, H1 does not appear to have propensity to adopt β-strand conformation or at least to unfold under its own thermal vibration. The salt bridges (SB1: R919-D1042, SB2: D922-R1042) between H1 tail and H4 have been suggested, among other factors, to hold H1 to the bundle. However, these two salt bridges are frequently broken which means they are not the key in holding H1 to the bundle. Moreover, in the absence of both LD motifs, H1 is strongly attached to the bundle and remains folded, so the LD motifs do not appear to affect the stability of the FAT domain. The isolated H1 simulation shows that H1 has the propensity to unfold from its C-terminal, keeping in mind that Y925 is located at the N-terminal. The C-terminal of H1 connects to a hinge region (contains two proline residues) that has been suggested to have the ability to promote such H1 unfolding from its C-terminal. In the isolated LD4 simulation, LD motif does have the capacity to keep its helical character. However, in literature, it has been assumed to be in helical form in nature. In summary, under only thermal fluctuation, H1 does not demonstrate the capacity to undergo the required structural rearrangement needed for Y925 phosphorylation. This result, besides the fact that FAK is hypothesized to be mechanically activated, are motivations to examine the influence of the applied load on H1 behavior.

Two applied mechanical load scenarios were chosen: axial and perpendicular. For the constrained axial load scenario, a 100 pN constant load was applied to the N-terminus of H1 tail in a direction parallel to the H1 axis and in the presence of both constrained P1 and P2 which are constrained. This load scenario was chosen based on the assumption

that axial load direction should most efficiently unravel H1. For the perpendicular load scenario, the same load was applied to the N-terminus of H1 in a direction perpendicular to the P1 axis but in the presence of P1 only. This load scenario was chosen based on the idea that P2, which blocks the access to Y925, has to first leave in order for the perpendicular load to open the FAT domain. The total loaded simulation time for the two load scenarios (axial and perpendicular) is 620 ns.

5.2 Under Axial Load, Y925 Phosphorylation Conditions Not Met

Under axial load, CFMD simulations show high propensity of H1 to stay folded and highly attached. Moreover, the salt bridges do not appear to have an influence on H1 position or H1 unfolding since they are broken most of the time. Also, the second salt bridge (SB2: D922-R1042) persists longer under the load influence, than in equilibrium, in which it is weaker. This suggests that the interactions found in the crystal structure may not persist in the dynamic in vivo environment. Load may play role in either breaking or supporting the salt bridges. Even by applying 100 pN for a total of 200 ns long, there is no simulation that H1 undergo the hypothesized structure of the FAT domain in which H1 is out of the bundle and the area flanking Y925 adopts a β-strand conformation.

5.3 Under Perpendicular Load, Y925 Phosphorylation Conditions Not Met

Perpendicular load simulations also show high propensity of H1 to be attached to the bundle as well as retain its helical form. In addition, the salt bridges do not appear to have an influence on H1unfolding or the H1 position, as has been found in

axial load scenario. Under either perpendicular or axial load, the behavior of the salt bridges is similar. After applying a 100 pN (in either the axial or perpendicular direction), for a cumulative total of 240 ns long, only one simulation out of 12 simulations adopts the hypothesized structure in which H1 is out of the bundle and the area flanking Y925 adopts a complete β-strand conformation. As a result, nine more simulations were run in which they have the same initial structure (as the one that undergoes the needed structural conformation changes for Y925 phosphorylation) but each with different initial velocities. These simulations were run to examine the repeatability of this type of behavior. However, this type of behavior, where H1 is highly attached to the bundle and it does not have a propensity to unfold, wes not found to be repeatable. Moreover, one of these nine simulations, the FAT is pulled away from the paxillin, raising the question of how much load the FAT/paxillin interactions can carry. In the future work, it will be important to examine the strength of the interaction between FAT and paxillin.

5.4 Mechanical Load is Insufficient Over the Examined Timescales

All the results suggest that either the mechanical load alone is insufficient to make Y925 accessible for phosphorylation or it is a very slow process. Furthermore, it might be something more than load has to take place for making Y925 accessible for phosphorylation such as chemical interactions. This could be a good motivation for looking for other factors that could contribute in getting Y925 available for phosphorylation.

Chapter 6. Future Work

From equilibrium and loading simulations, it appears that H1 has very high propensity to stay folded within the bundle. It has been reported that Y925, located in the N-terminal of the first helix (H1) of FAT, is phosphorylated. However, this suggests that either this kind of process takes a long time or/and different conditions have to occur.

Longer CFMD simulations (more than 20 ns each) should be run to assess the time required for H1 to undergo that the structural changes needed for Y925 phosphorylation. Along the line with the necessity of extending the CFMD simulations, the unfolding propagation, if any, will be investigated via "satates" and net fluxes between states. The hydrogen donor-acceptor pairs and the ψ dihedral angle of the first five residues of the N-terminal of H1 (including Y925) will be key states. These calculations generate the possible states that the region flanking Y925 occupies, which gives a specific assessment of the unfolding initiation and propagation that could occur.

Since only two load scenarios (axial and perpendicular) with one load level (100 pN) were considered, different load directions with different load levels should be considered in any additional CFMD simulations. It may be that the most realistic load scenario is more complicated than the simple ones examined in this study. So, it is important to make the load scenarios as realistic as possible. As a result, constraining the ends of LD motifs, for example, should re-examined. In addition, for physiological reasons, lower load levels should be examined.

The strength of all possible interactions (electrostatic and hydrophobic) between H1 and the neighbor helices, including LD motifs, should be evaluated as a function of the applied load. Correlations between the strength of these interactions and the

availability of Y925 should be calculated. This will give a better understanding of the key regulators as they may gate of the Y925 phosphorylation.

H1/H2 hinge has been suggested to have a role in promoting the structural changes needed for Y925 phosphorylation. Moreover, MD simulation of the isolated H1 shows that H1 has a propensity to unfold from its C-terminal, which is one arm of the H1/H2 hinge. It is possible that H1 may unfold from its C-terminal and not from the N-terminal (where Y925 located). So, it is important to investigate the behavior of H1's C-terminal residues. To accomplish, the ψ dihedral angle and hydrogen donor-acceptor pairs states will be examined.

Appendix A. PDB Files

1. The FAT/paxillin complex constructed using raw file 1ow7.pdb (§3.1.1 Structures):

```
HEADER    TRANSFERASE                             28-MAR-03   1OW7
TITLE     PAXILLIN LD4 MOTIF BOUND TO THE FOCAL ADHESION TARGETING
TITLE    2 (FAT) DOMAIN OF THE FOCAL ADHESION KINASE
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: FOCAL ADHESION KINASE 1;
COMPND   3 CHAIN: A, B, C;
COMPND   4 FRAGMENT: FOCAL ADHESION TARGETING DOMAIN;
COMPND   5 SYNONYM: FADK 1, PP125FAK, PROTEIN- TYROSINE KINASE 2;
COMPND   6 EC: 2.7.1.112;
COMPND   7 ENGINEERED: YES;
COMPND   8 MOL_ID: 2;
COMPND   9 MOLECULE: PAXILLIN;
COMPND  10 CHAIN: D, E, F;
COMPND  11 FRAGMENT: PAXILLIN LD4 MOTIF;
COMPND  12 ENGINEERED: YES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE   3 ORGANISM_COMMON: HUMAN;
SOURCE   4 ORGANISM_TAXID: 9606;
SOURCE   5 GENE: PTK2 OR FAK1 OR FAK;
SOURCE   6 EXPRESSION_SYSTEM: ESCHERICHIA COLI BL21(DE3);
SOURCE   7 EXPRESSION_SYSTEM_TAXID: 469008;
SOURCE   8 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE   9 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE  10 EXPRESSION_SYSTEM_PLASMID: PGEX-6P2;
SOURCE  11 MOL_ID: 2;
SOURCE  12 SYNTHETIC: YES;
SOURCE  13 OTHER_DETAILS: SEQUENCE DERIVED FROM HUMAN PAXILLIN
KEYWDS    4 HELICAL BUNDLE, AMPHIPHATIC HELIX, TRANSFERASE
EXPDTA    X-RAY DIFFRACTION
```

```
AUTHOR    M.K.HOELLERER,M.E.M.NOBLE,G.LABESSE,J.M.WERNER,S.T.AROLD
REVDAT   2   24-FEB-09 1OW7    1       VERSN
REVDAT   1   21-OCT-03 1OW7    0
JRNL        AUTH   M.K.HOELLERER,M.E.M.NOBLE,G.LABESSE,J.M.WERNER,
JRNL        AUTH 2 S.T.AROLD
JRNL        TITL   MOLECULAR RECOGNITION OF PAXILLIN LD MOTIFS BY THE
JRNL        TITL 2 FOCAL ADHESION TARGETING DOMAIN
JRNL        REF    STRUCTURE                     V.  11  1207 2003
JRNL        REFN                   ISSN 0969-2126
JRNL        PMID   14527389
JRNL        DOI    10.1016/J.STR.2003.08.010
REMARK   1
REMARK   2
REMARK   2 RESOLUTION.    2.60 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC 5.1.24
REMARK   3   AUTHORS     : MURSHUDOV,VAGIN,DODSON
REMARK   3
REMARK   3    REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 2.60
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 111.80
REMARK   3   DATA CUTOFF            (SIGMA(F)) : 0.000
REMARK   3   COMPLETENESS FOR RANGE        (%) : 78.2
REMARK   3   NUMBER OF REFLECTIONS             : 23071
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD          : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION  : RANDOM
REMARK   3   R VALUE     (WORKING + TEST SET) : 0.239
REMARK   3   R VALUE            (WORKING SET) : 0.237
REMARK   3   FREE R VALUE                     : 0.269
REMARK   3   FREE R VALUE TEST SET SIZE   (%) : 5.200
REMARK   3   FREE R VALUE TEST SET COUNT      : 1189
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           : 20
```

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REMARK   3   BIN RESOLUTION RANGE HIGH       (A) : 2.60
REMARK   3   BIN RESOLUTION RANGE LOW        (A) : 2.67
REMARK   3   REFLECTION IN BIN     (WORKING SET) : 785
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REMARK   3   BIN R VALUE           (WORKING SET) : 0.4350
REMARK   3   BIN FREE R VALUE SET COUNT          : 48
REMARK   3   BIN FREE R VALUE                    : 0.4630
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 3470
REMARK   3   NUCLEIC ACID ATOMS       : 0
REMARK   3   HETEROGEN ATOMS          : 0
REMARK   3   SOLVENT ATOMS            : 50
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : 76.00
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : 74.70
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) : 7.65000
REMARK   3    B22 (A**2) : -3.19000
REMARK   3    B33 (A**2) : -4.46000
REMARK   3    B12 (A**2) : 0.00000
REMARK   3    B13 (A**2) : 0.00000
REMARK   3    B23 (A**2) : 0.00000
REMARK   3
REMARK   3  ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3   ESU BASED ON R VALUE                            (A): 0.460
REMARK   3   ESU BASED ON FREE R VALUE                       (A): 0.311
REMARK   3   ESU BASED ON MAXIMUM LIKELIHOOD                 (A): NULL
REMARK   3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): NULL
REMARK   3
REMARK   3 CORRELATION COEFFICIENTS.
REMARK   3   CORRELATION COEFFICIENT FO-FC      : 0.935
REMARK   3   CORRELATION COEFFICIENT FO-FC FREE : 0.909
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES        COUNT    RMS    WEIGHT
REMARK   3   BOND LENGTHS REFINED ATOMS        (A):  3509 ; 0.012 ; 0.022
REMARK   3   BOND LENGTHS OTHERS               (A):  3367 ; 0.000 ; 0.020
REMARK   3   BOND ANGLES REFINED ATOMS   (DEGREES):  4744 ; 1.713 ; 2.010
```

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REMARK   3   BOND ANGLES OTHERS          (DEGREES):  7895 ; 3.480 ; 3.000
REMARK   3   TORSION ANGLES, PERIOD 1    (DEGREES):   442 ; 1.430 ; 5.000
REMARK   3   TORSION ANGLES, PERIOD 2    (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   TORSION ANGLES, PERIOD 3    (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   TORSION ANGLES, PERIOD 4    (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   CHIRAL-CENTER RESTRAINTS       (A**3):   585 ; 0.112 ; 0.200
REMARK   3   GENERAL PLANES REFINED ATOMS      (A):  3761 ; 0.008 ; 0.020
REMARK   3   GENERAL PLANES OTHERS             (A):   538 ; 0.005 ; 0.020
REMARK   3   NON-BONDED CONTACTS REFINED ATOMS (A):  1038 ; 0.251 ; 0.200
REMARK   3   NON-BONDED CONTACTS OTHERS        (A):  3922 ; 0.294 ; 0.200
REMARK   3   NON-BONDED TORSION REFINED ATOMS  (A):  NULL ;  NULL ;  NULL
REMARK   3   NON-BONDED TORSION OTHERS         (A):  1835 ; 0.107 ; 0.200
REMARK   3   H-BOND (X...Y) REFINED ATOMS      (A):    57 ; 0.174 ; 0.200
REMARK   3   H-BOND (X...Y) OTHERS             (A):  NULL ;  NULL ;  NULL
REMARK   3   POTENTIAL METAL-ION REFINED ATOMS (A):  NULL ;  NULL ;  NULL
REMARK   3   POTENTIAL METAL-ION OTHERS        (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY VDW REFINED ATOMS        (A):    15 ; 0.278 ; 0.200
REMARK   3   SYMMETRY VDW OTHERS               (A):    73 ; 0.309 ; 0.200
REMARK   3   SYMMETRY H-BOND REFINED ATOMS     (A):     5 ; 0.142 ; 0.200
REMARK   3   SYMMETRY H-BOND OTHERS            (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY METAL-ION REFINED ATOMS  (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY METAL-ION OTHERS         (A):  NULL ;  NULL ;  NULL
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.     COUNT   RMS    WEIGHT
REMARK   3   MAIN-CHAIN BOND REFINED ATOMS  (A**2):  2252 ; 2.828 ; 1.500
REMARK   3   MAIN-CHAIN BOND OTHER ATOMS    (A**2):  NULL ;  NULL ;  NULL
REMARK   3   MAIN-CHAIN ANGLE REFINED ATOMS (A**2):  3644 ; 5.037 ; 2.000
REMARK   3   SIDE-CHAIN BOND REFINED ATOMS  (A**2):  1257 ; 4.743 ; 3.000
REMARK   3   SIDE-CHAIN ANGLE REFINED ATOMS (A**2):  1100 ; 7.598 ; 4.500
REMARK   3
REMARK   3 ANISOTROPIC THERMAL FACTOR RESTRAINTS.    COUNT   RMS   WEIGHT
REMARK   3   RIGID-BOND RESTRAINTS          (A**2):  NULL ;  NULL ;  NULL
REMARK   3   SPHERICITY; FREE ATOMS         (A**2):  NULL ;  NULL ;  NULL
REMARK   3   SPHERICITY; BONDED ATOMS       (A**2):  NULL ;  NULL ;  NULL
REMARK   3
REMARK   3  NCS RESTRAINTS STATISTICS
REMARK   3   NUMBER OF DIFFERENT NCS GROUPS : NULL
REMARK   3
REMARK   3  TLS DETAILS
```

```
REMARK   3   NUMBER OF TLS GROUPS  : NULL
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3   METHOD USED : BABINET MODEL WITH MASK
REMARK   3   PARAMETERS FOR MASK CALCULATION
REMARK   3   VDW PROBE RADIUS   : 1.40
REMARK   3   ION PROBE RADIUS   : 0.80
REMARK   3   SHRINKAGE RADIUS   : 0.80
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: 1) THE SECOND LD4 MOTIF (CHAIN F,
REMARK   3  BOUND TO MOLECULE C) WAS FITTED INTO THE UNBIASED 3FO-2FC MAPS
REMARK   3  (CNS). ITS POSITION AND ORIENTATION WERE INFERRED FROM
REMARK   3  HOMOLOGY WITH THE WELL-DEFINED OTHER LD4 - FAT INTERACTION
REMARK   3  (CHAINS A AND C), AND ARE SUPPORTED BY NMR DATA(SEE
REMARK   3  PUBLICATION). 2) THE CRYSTAL DIFFRACTED ANISOTROPICALLY TO 2.8
REMARK   3  AND 2.6 A RESOLUTION. THE WEAK, BUT CONSISTENT, DATA TO 2.6 A
REMARK   3  WERE INCLUDED, AS THEY SIGNIFICANTLY IMPROVED THE ELECTRON
REMARK   3  DENSITY.
REMARK   4
REMARK   4 1OW7 COMPLIES WITH FORMAT V. 3.15, 01-DEC-08
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 31-MAR-03.
REMARK 100 THE RCSB ID CODE IS RCSB018728.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : 30-JUN-02
REMARK 200  TEMPERATURE           (KELVIN) : 100
REMARK 200  PH                             : 6.3
REMARK 200  NUMBER OF CRYSTALS USED        : 1
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : Y
REMARK 200  RADIATION SOURCE               : ESRF
REMARK 200  BEAMLINE                       : BM30A
REMARK 200  X-RAY GENERATOR MODEL          : NULL
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : M
REMARK 200  WAVELENGTH OR RANGE        (A) : 0.98
REMARK 200  MONOCHROMATOR                  : SILICON
REMARK 200  OPTICS                         : TWO CRYSTALS MONOCHROMATOR
```

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REMARK 200                                   BETWEEN TWO CYLINDRICAL
REMARK 200                                   PARABOLIC MIRRORS
REMARK 200
REMARK 200  DETECTOR TYPE                  : CCD
REMARK 200  DETECTOR MANUFACTURER          : MARRESEARCH
REMARK 200  INTENSITY-INTEGRATION SOFTWARE : MOSFLM
REMARK 200  DATA SCALING SOFTWARE          : CCP4 (SCALA)
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 23071
REMARK 200  RESOLUTION RANGE HIGH      (A) : 2.600
REMARK 200  RESOLUTION RANGE LOW       (A) : 29.600
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : NULL
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%) : 88.7
REMARK 200  DATA REDUNDANCY                : 2.700
REMARK 200  R MERGE                    (I) : 0.07900
REMARK 200  R SYM                      (I) : 0.06400
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET  : 8.9000
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.60
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.69
REMARK 200  COMPLETENESS FOR SHELL     (%) : 79.3
REMARK 200  DATA REDUNDANCY IN SHELL       : 1.70
REMARK 200  R MERGE FOR SHELL          (I) : 0.86000
REMARK 200  R SYM FOR SHELL            (I) : 0.62000
REMARK 200  <I/SIGMA(I)> FOR SHELL         : 0.300
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
REMARK 200 SOFTWARE USED: AMORE
REMARK 200 STARTING MODEL: PDBENTRY 1K05
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): 74.01
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 4.77
```

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REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: SODIUM CHLORIDE, GLYCEROL, HEPES,
REMARK 280  PH 6.3, VAPOR DIFFUSION, HANGING DROP, TEMPERATURE 292K
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: C 2 2 21
REMARK 290
REMARK 290      SYMOP   SYMMETRY
REMARK 290     NNNMMM   OPERATOR
REMARK 290       1555   X,Y,Z
REMARK 290       2555   -X,-Y,Z+1/2
REMARK 290       3555   -X,Y,-Z+1/2
REMARK 290       4555   X,-Y,-Z
REMARK 290       5555   X+1/2,Y+1/2,Z
REMARK 290       6555   -X+1/2,-Y+1/2,Z+1/2
REMARK 290       7555   -X+1/2,Y+1/2,-Z+1/2
REMARK 290       8555   X+1/2,-Y+1/2,-Z
REMARK 290
REMARK 290     WHERE NNN -> OPERATOR NUMBER
REMARK 290           MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290   SMTRY1   1  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   2 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   2  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   2  0.000000  0.000000  1.000000       48.09950
REMARK 290   SMTRY1   3 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   3  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   3  0.000000  0.000000 -1.000000       48.09950
REMARK 290   SMTRY1   4  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   4  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   4  0.000000  0.000000 -1.000000        0.00000
REMARK 290   SMTRY1   5  1.000000  0.000000  0.000000       44.49700
REMARK 290   SMTRY2   5  0.000000  1.000000  0.000000      109.83250
```

```
REMARK 290   SMTRY3   5  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   6 -1.000000  0.000000  0.000000       44.49700
REMARK 290   SMTRY2   6  0.000000 -1.000000  0.000000      109.83250
REMARK 290   SMTRY3   6  0.000000  0.000000  1.000000       48.09950
REMARK 290   SMTRY1   7 -1.000000  0.000000  0.000000       44.49700
REMARK 290   SMTRY2   7  0.000000  1.000000  0.000000      109.83250
REMARK 290   SMTRY3   7  0.000000  0.000000 -1.000000       48.09950
REMARK 290   SMTRY1   8  1.000000  0.000000  0.000000       44.49700
REMARK 290   SMTRY2   8  0.000000 -1.000000  0.000000      109.83250
REMARK 290   SMTRY3   8  0.000000  0.000000 -1.000000        0.00000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 SEE REMARK 350 FOR THE AUTHOR PROVIDED AND/OR PROGRAM
REMARK 300 GENERATED ASSEMBLY INFORMATION FOR THE STRUCTURE IN
REMARK 300 THIS ENTRY. THE REMARK MAY ALSO PROVIDE INFORMATION ON
REMARK 300 BURIED SURFACE AREA.
REMARK 350
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: HEXAMERIC
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, B, C, D, E, F
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000        0.00000
REMARK 375
REMARK 375 SPECIAL POSITION
REMARK 375 THE FOLLOWING ATOMS ARE FOUND TO BE WITHIN 0.15 ANGSTROMS
REMARK 375 OF A SYMMETRY RELATED ATOM AND ARE ASSUMED TO BE ON SPECIAL
REMARK 375 POSITIONS.
REMARK 375
REMARK 375 ATOM RES CSSEQI
REMARK 375      HOH B  60  LIES ON A SPECIAL POSITION.
```

```
REMARK 375      HOH C   4  LIES ON A SPECIAL POSITION.
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465   M RES C SSSEQI
REMARK 465     SER A   892
REMARK 465     SER A   893
REMARK 465     PRO A   894
REMARK 465     ALA A   895
REMARK 465     ASP A   896
REMARK 465     SER A   897
REMARK 465     TYR A   898
REMARK 465     ASN A   899
REMARK 465     GLU A   900
REMARK 465     GLY A   901
REMARK 465     VAL A   902
REMARK 465     LYS A   903
REMARK 465     LEU A   904
REMARK 465     GLN A   905
REMARK 465     PRO A   906
REMARK 465     GLN A   907
REMARK 465     GLU A   908
REMARK 465     ILE A   909
REMARK 465     SER A   910
REMARK 465     PRO A   911
REMARK 465     PRO A   912
REMARK 465     PRO A   913
REMARK 465     THR A   914
REMARK 465     ALA A   915
REMARK 465     ARG A  1050
REMARK 465     PRO A  1051
REMARK 465     HIS A  1052
REMARK 465     SER B   892
REMARK 465     SER B   893
REMARK 465     PRO B   894
REMARK 465     ALA B   895
```

```
REMARK 465     ASP B   896
REMARK 465     SER B   897
REMARK 465     TYR B   898
REMARK 465     ASN B   899
REMARK 465     GLU B   900
REMARK 465     GLY B   901
REMARK 465     VAL B   902
REMARK 465     LYS B   903
REMARK 465     LEU B   904
REMARK 465     GLN B   905
REMARK 465     PRO B   906
REMARK 465     GLN B   907
REMARK 465     GLU B   908
REMARK 465     GLN B  1048
REMARK 465     THR B  1049
REMARK 465     ARG B  1050
REMARK 465     PRO B  1051
REMARK 465     HIS B  1052
REMARK 465     SER C   892
REMARK 465     SER C   893
REMARK 465     PRO C   894
REMARK 465     ALA C   895
REMARK 465     ASP C   896
REMARK 465     SER C   897
REMARK 465     TYR C   898
REMARK 465     ASN C   899
REMARK 465     GLU C   900
REMARK 465     GLY C   901
REMARK 465     VAL C   902
REMARK 465     LYS C   903
REMARK 465     LEU C   904
REMARK 465     GLN C   905
REMARK 465     PRO C   906
REMARK 465     GLN C   907
REMARK 465     GLU C   908
REMARK 465     GLN C  1048
REMARK 465     THR C  1049
REMARK 465     ARG C  1050
REMARK 465     PRO C  1051
```

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REMARK 465     HIS C  1052
REMARK 465     ALA D     1
REMARK 465     ALA E     1
REMARK 465     ALA F     1
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: TORSION ANGLES
REMARK 500
REMARK 500 TORSION ANGLES OUTSIDE THE EXPECTED RAMACHANDRAN REGIONS:
REMARK 500 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER;
REMARK 500 SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT:(10X,I3,1X,A3,1X,A1,I4,A1,4X,F7.2,3X,F7.2)
REMARK 500
REMARK 500 EXPECTED VALUES: GJ KLEYWEGT AND TA JONES (1996). PHI/PSI-
REMARK 500 CHOLOGY: RAMACHANDRAN REVISITED. STRUCTURE 4, 1395 - 1400
REMARK 500
REMARK 500  M RES CSSEQI        PSI       PHI
REMARK 500    SER A 920      -39.71    -39.13
REMARK 500    TYR A1007       32.90    -91.74
REMARK 500    MET A1009       13.73     81.75
REMARK 500    MET B1009       -3.32     72.96
REMARK 500    ASN C 916       21.89    -71.05
REMARK 500    LYS C 941      -94.67    -97.28
REMARK 500    ILE C 942      -47.69      4.76
REMARK 500    PRO C 944      -78.50    -55.50
REMARK 500    ALA C 945      142.87    -29.64
REMARK 500    TYR C1016       -1.48    -56.86
REMARK 500
REMARK 500 REMARK: NULL
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1K05   RELATED DB: PDB
REMARK 900 CRYSTAL STRUCTURE OF THE FOCAL ADHESION TARGETING DOMAIN OF
REMARK 900 FOCAL ADHESION KINASE
DBREF  1OW7 A  892  1052  UNP    Q05397   FAK1_HUMAN     892   1052
DBREF  1OW7 B  892  1052  UNP    Q05397   FAK1_HUMAN     892   1052
DBREF  1OW7 C  892  1052  UNP    Q05397   FAK1_HUMAN     892   1052
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DBREF  1OW7 D    1    13  PDB    1OW7     1OW7             1     13
DBREF  1OW7 E    1    13  PDB    1OW7     1OW7             1     13
DBREF  1OW7 F    1    13  PDB    1OW7     1OW7             1     13
SEQRES   1 A  161  SER SER PRO ALA ASP SER TYR ASN GLU GLY VAL LYS LEU
SEQRES   2 A  161  GLN PRO GLN GLU ILE SER PRO PRO PRO THR ALA ASN LEU
SEQRES   3 A  161  ASP ARG SER ASN ASP LYS VAL TYR GLU ASN VAL THR GLY
SEQRES   4 A  161  LEU VAL LYS ALA VAL ILE GLU MET SER SER LYS ILE GLN
SEQRES   5 A  161  PRO ALA PRO PRO GLU GLU TYR VAL PRO MET VAL LYS GLU
SEQRES   6 A  161  VAL GLY LEU ALA LEU ARG THR LEU LEU ALA THR VAL ASP
SEQRES   7 A  161  GLU THR ILE PRO LEU LEU PRO ALA SER THR HIS ARG GLU
SEQRES   8 A  161  ILE GLU MET ALA GLN LYS LEU LEU ASN SER ASP LEU GLY
SEQRES   9 A  161  GLU LEU ILE ASN LYS MET LYS LEU ALA GLN GLN TYR VAL
SEQRES  10 A  161  MET THR SER LEU GLN GLN GLU TYR LYS LYS GLN MET LEU
SEQRES  11 A  161  THR ALA ALA HIS ALA LEU ALA VAL ASP ALA LYS ASN LEU
SEQRES  12 A  161  LEU ASP VAL ILE ASP GLN ALA ARG LEU LYS MET LEU GLY
SEQRES  13 A  161  GLN THR ARG PRO HIS
SEQRES   1 B  161  SER SER PRO ALA ASP SER TYR ASN GLU GLY VAL LYS LEU
SEQRES   2 B  161  GLN PRO GLN GLU ILE SER PRO PRO PRO THR ALA ASN LEU
SEQRES   3 B  161  ASP ARG SER ASN ASP LYS VAL TYR GLU ASN VAL THR GLY
SEQRES   4 B  161  LEU VAL LYS ALA VAL ILE GLU MET SER SER LYS ILE GLN
SEQRES   5 B  161  PRO ALA PRO PRO GLU GLU TYR VAL PRO MET VAL LYS GLU
SEQRES   6 B  161  VAL GLY LEU ALA LEU ARG THR LEU LEU ALA THR VAL ASP
SEQRES   7 B  161  GLU THR ILE PRO LEU LEU PRO ALA SER THR HIS ARG GLU
SEQRES   8 B  161  ILE GLU MET ALA GLN LYS LEU LEU ASN SER ASP LEU GLY
SEQRES   9 B  161  GLU LEU ILE ASN LYS MET LYS LEU ALA GLN GLN TYR VAL
SEQRES  10 B  161  MET THR SER LEU GLN GLN GLU TYR LYS LYS GLN MET LEU
SEQRES  11 B  161  THR ALA ALA HIS ALA LEU ALA VAL ASP ALA LYS ASN LEU
SEQRES  12 B  161  LEU ASP VAL ILE ASP GLN ALA ARG LEU LYS MET LEU GLY
SEQRES  13 B  161  GLN THR ARG PRO HIS
SEQRES   1 C  161  SER SER PRO ALA ASP SER TYR ASN GLU GLY VAL LYS LEU
SEQRES   2 C  161  GLN PRO GLN GLU ILE SER PRO PRO PRO THR ALA ASN LEU
SEQRES   3 C  161  ASP ARG SER ASN ASP LYS VAL TYR GLU ASN VAL THR GLY
SEQRES   4 C  161  LEU VAL LYS ALA VAL ILE GLU MET SER SER LYS ILE GLN
SEQRES   5 C  161  PRO ALA PRO PRO GLU GLU TYR VAL PRO MET VAL LYS GLU
SEQRES   6 C  161  VAL GLY LEU ALA LEU ARG THR LEU LEU ALA THR VAL ASP
SEQRES   7 C  161  GLU THR ILE PRO LEU LEU PRO ALA SER THR HIS ARG GLU
SEQRES   8 C  161  ILE GLU MET ALA GLN LYS LEU LEU ASN SER ASP LEU GLY
SEQRES   9 C  161  GLU LEU ILE ASN LYS MET LYS LEU ALA GLN GLN TYR VAL
SEQRES  10 C  161  MET THR SER LEU GLN GLN GLU TYR LYS LYS GLN MET LEU
```

```
SEQRES  11 C  161  THR ALA ALA HIS ALA LEU ALA VAL ASP ALA LYS ASN LEU
SEQRES  12 C  161  LEU ASP VAL ILE ASP GLN ALA ARG LEU LYS MET LEU GLY
SEQRES  13 C  161  GLN THR ARG PRO HIS
SEQRES   1 D   13  ALA THR ARG GLU LEU ASP GLU LEU MET ALA SER LEU SER
SEQRES   1 E   13  ALA THR ARG GLU LEU ASP GLU LEU MET ALA SER LEU SER
SEQRES   1 F   13  ALA THR ARG GLU LEU ASP GLU LEU MET ALA SER LEU SER
FORMUL   7  HOH   *50(H2 O)
HELIX    1   1 ASP A  922  ILE A  942  1                                  21
HELIX    2   2 PRO A  946  ILE A  972  1                                  27
HELIX    3   3 PRO A  973  LEU A  975  5                                   3
HELIX    4   4 THR A  979  TYR A 1007  1                                  29
HELIX    5   5 LEU A 1012  GLY A 1047  1                                  36
HELIX    6   6 ASP B  922  ILE B  942  1                                  21
HELIX    7   7 PRO B  946  GLU B  970  1                                  25
HELIX    8   8 THR B  971  LEU B  975  5                                   5
HELIX    9   9 PRO B  976  SER B  978  5                                   3
HELIX   10  10 THR B  979  TYR B 1007  1                                  29
HELIX   11  11 SER B 1011  LEU B 1046  1                                  36
HELIX   12  12 ASP C  922  LYS C  941  1                                  20
HELIX   13  13 PRO C  946  ILE C  972  1                                  27
HELIX   14  14 THR C  979  TYR C 1007  1                                  29
HELIX   15  15 THR C 1010  GLY C 1047  1                                  38
HELIX   16  16 GLU D    4  LEU D   12  1                                   9
HELIX   17  17 GLU E    4  ALA E   10  1                                   7
HELIX   18  18 THR F    2  LEU F   12  1                                  11
CRYST1   88.994  219.665   96.199  90.00  90.00  90.00 C 2 2 21     24
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.011237  0.000000  0.000000        0.00000
SCALE2      0.000000  0.004552  0.000000        0.00000
SCALE3      0.000000  0.000000  0.010395        0.00000
ATOM     12  N   ILE C 909      -7.120  90.264  27.594  1.00 84.95           N
ATOM     13  CA  ILE C 909      -6.328  91.240  26.773  1.00 86.58           C
ATOM     14  C   ILE C 909      -6.742  92.707  26.925  1.00 85.87           C
ATOM     15  O   ILE C 909      -7.924  93.047  26.881  1.00 86.73           O
ATOM     16  CB  ILE C 909      -6.375  90.883  25.252  1.00 85.93           C
ATOM     17  CG1 ILE C 909      -5.547  91.908  24.460  1.00 84.17           C
ATOM     18  CG2 ILE C 909      -7.829  90.811  24.763  1.00 79.59           C
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ATOM     19  CD1 ILE C 909      -5.233  91.508  23.026  1.00 82.55           C
ATOM     20  N   SER C 910      -5.760  93.584  27.092  1.00 85.82           N
ATOM     21  CA  SER C 910      -6.064  95.004  27.245  1.00 88.03           C
ATOM     22  C   SER C 910      -6.002  95.773  25.931  1.00 87.92           C
ATOM     23  O   SER C 910      -5.363  95.336  24.962  1.00 90.37           O
ATOM     24  CB  SER C 910      -5.117  95.644  28.260  1.00 87.19           C
ATOM     25  OG  SER C 910      -3.892  94.924  28.339  1.00 88.96           O
ATOM     26  N   PRO C 911      -6.707  96.919  25.869  1.00 85.92           N
ATOM     27  CA  PRO C 911      -6.692  97.727  24.649  1.00 82.06           C
ATOM     28  C   PRO C 911      -5.458  98.621  24.779  1.00 76.36           C
ATOM     29  O   PRO C 911      -4.891  98.763  25.878  1.00 72.62           O
ATOM     30  CB  PRO C 911      -8.003  98.513  24.750  1.00 81.26           C
ATOM     31  CG  PRO C 911      -8.052  98.813  26.204  1.00 83.81           C
ATOM     32  CD  PRO C 911      -7.705  97.441  26.818  1.00 84.68           C
ATOM     33  N   PRO C 912      -5.029  99.238  23.668  1.00 69.40           N
ATOM     34  CA  PRO C 912      -3.851 100.103  23.695  1.00 63.70           C
ATOM     35  C   PRO C 912      -3.917 101.091  24.857  1.00 60.56           C
ATOM     36  O   PRO C 912      -4.996 101.538  25.235  1.00 61.26           O
ATOM     37  CB  PRO C 912      -3.923 100.804  22.338  1.00 65.28           C
ATOM     38  CG  PRO C 912      -4.655  99.848  21.490  1.00 64.22           C
ATOM     39  CD  PRO C 912      -5.745  99.375  22.395  1.00 65.66           C
ATOM     40  N   PRO C 913      -2.763 101.438  25.446  1.00 58.77           N
ATOM     41  CA  PRO C 913      -2.797 102.386  26.571  1.00 61.24           C
ATOM     42  C   PRO C 913      -3.755 103.530  26.256  1.00 63.36           C
ATOM     43  O   PRO C 913      -3.840 103.956  25.109  1.00 67.19           O
ATOM     44  CB  PRO C 913      -1.349 102.849  26.685  1.00 59.78           C
ATOM     45  CG  PRO C 913      -0.577 101.661  26.222  1.00 59.63           C
ATOM     46  CD  PRO C 913      -1.386 101.084  25.074  1.00 59.35           C
ATOM     47  N   THR C 914      -4.458 104.042  27.266  1.00 65.08           N
ATOM     48  CA  THR C 914      -5.436 105.093  27.011  1.00 69.04           C
ATOM     49  C   THR C 914      -4.815 106.370  26.491  1.00 73.88           C
ATOM     50  O   THR C 914      -3.717 106.786  26.919  1.00 72.02           O
ATOM     51  CB  THR C 914      -6.315 105.419  28.250  1.00 69.24           C
ATOM     52  CG2 THR C 914      -5.485 106.060  29.340  1.00 69.56           C
ATOM     53  OG1 THR C 914      -7.361 106.329  27.874  1.00 67.64           O
ATOM     54  N   ALA C 915      -5.531 106.964  25.535  1.00 76.34           N
ATOM     55  CA  ALA C 915      -5.106 108.193  24.885  1.00 78.39           C
ATOM     56  C   ALA C 915      -5.407 109.387  25.786  1.00 81.78           C
ATOM     57  O   ALA C 915      -4.725 110.418  25.718  1.00 84.63           O
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ATOM     58  CB  ALA C 915      -5.821 108.341  23.538  1.00 73.31           C
ATOM     59  N   ASN C 916      -6.399 109.226  26.660  1.00 82.80           N
ATOM     60  CA  ASN C 916      -6.816 110.305  27.546  1.00 82.11           C
ATOM     61  C   ASN C 916      -5.834 110.665  28.679  1.00 79.48           C
ATOM     62  O   ASN C 916      -6.252 111.247  29.670  1.00 75.73           O
ATOM     63  CB  ASN C 916      -8.204 109.979  28.131  1.00 88.81           C
ATOM     64  CG  ASN C 916      -9.073 109.113  27.184  1.00 94.91           C
ATOM     65  ND2 ASN C 916      -9.575 107.988  27.704  1.00 96.94           N
ATOM     66  OD1 ASN C 916      -9.289 109.455  26.012  1.00 99.35           O
ATOM     67  N   LEU C 917      -4.549 110.328  28.531  1.00 76.82           N
ATOM     68  CA  LEU C 917      -3.513 110.651  29.529  1.00 76.15           C
ATOM     69  C   LEU C 917      -2.212 111.089  28.847  1.00 76.67           C
ATOM     70  O   LEU C 917      -1.728 110.419  27.941  1.00 78.80           O
ATOM     71  CB  LEU C 917      -3.179 109.444  30.403  1.00 78.46           C
ATOM     72  CG  LEU C 917      -4.159 108.769  31.351  1.00 80.00           C
ATOM     73  CD1 LEU C 917      -3.506 107.526  31.939  1.00 78.87           C
ATOM     74  CD2 LEU C 917      -4.546 109.731  32.447  1.00 85.50           C
ATOM     75  N   ASP C 918      -1.611 112.173  29.311  1.00 78.12           N
ATOM     76  CA  ASP C 918      -0.394 112.668  28.673  1.00 82.31           C
ATOM     77  C   ASP C 918       0.858 111.919  29.108  1.00 81.67           C
ATOM     78  O   ASP C 918       1.210 111.929  30.285  1.00 84.04           O
ATOM     79  CB  ASP C 918      -0.238 114.174  28.947  1.00 88.22           C
ATOM     80  CG  ASP C 918       1.043 114.760  28.347  1.00 94.03           C
ATOM     81  OD1 ASP C 918       2.096 114.097  28.473  1.00 98.43           O
ATOM     82  OD2 ASP C 918       1.002 115.882  27.776  1.00 97.26           O
ATOM     83  N   ARG C 919       1.552 111.315  28.140  1.00 77.81           N
ATOM     84  CA  ARG C 919       2.757 110.518  28.399  1.00 71.26           C
ATOM     85  C   ARG C 919       4.063 111.292  28.346  1.00 73.28           C
ATOM     86  O   ARG C 919       5.138 110.691  28.354  1.00 77.64           O
ATOM     87  CB  ARG C 919       2.842 109.384  27.386  1.00 60.42           C
ATOM     88  CG  ARG C 919       1.550 108.657  27.167  1.00 57.11           C
ATOM     89  CD  ARG C 919       1.107 107.962  28.421  1.00 54.34           C
ATOM     90  NE  ARG C 919      -0.182 107.321  28.226  1.00 57.02           N
ATOM     91  CZ  ARG C 919      -0.705 106.445  29.072  1.00 55.74           C
ATOM     92  NH1 ARG C 919      -0.039 106.116  30.173  1.00 54.16           N
ATOM     93  NH2 ARG C 919      -1.874 105.878  28.794  1.00 54.13           N
ATOM     94  N   SER C 920       3.984 112.613  28.284  1.00 74.38           N
ATOM     95  CA  SER C 920       5.195 113.421  28.187  1.00 76.74           C
ATOM     96  C   SER C 920       6.091 113.252  29.365  1.00 75.30           C
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ATOM     97  O   SER C 920       7.317 113.241  29.232  1.00 72.65           O
ATOM     98  CB  SER C 920       4.871 114.909  28.089  1.00 79.67           C
ATOM     99  OG  SER C 920       4.047 115.190  26.977  1.00 89.57           O
ATOM    100  N   ASN C 921       5.466 113.149  30.529  1.00 77.59           N
ATOM    101  CA  ASN C 921       6.220 113.042  31.761  1.00 80.00           C
ATOM    102  C   ASN C 921       5.910 111.775  32.547  1.00 79.61           C
ATOM    103  O   ASN C 921       6.108 111.720  33.763  1.00 83.99           O
ATOM    104  CB  ASN C 921       5.972 114.304  32.602  1.00 78.49           C
ATOM    105  CG  ASN C 921       6.493 115.567  31.912  1.00 79.04           C
ATOM    106  ND2 ASN C 921       5.604 116.532  31.661  1.00 74.33           N
ATOM    107  OD1 ASN C 921       7.684 115.660  31.596  1.00 79.77           O
ATOM    108  N   ASP C 922       5.440 110.756  31.831  1.00 73.79           N
ATOM    109  CA  ASP C 922       5.106 109.470  32.427  1.00 70.09           C
ATOM    110  C   ASP C 922       6.337 108.555  32.462  1.00 69.92           C
ATOM    111  O   ASP C 922       6.608 107.825  31.504  1.00 71.98           O
ATOM    112  CB  ASP C 922       3.996 108.781  31.630  1.00 65.82           C
ATOM    113  CG  ASP C 922       3.281 107.715  32.440  1.00 66.60           C
ATOM    114  OD1 ASP C 922       3.871 107.216  33.425  1.00 64.17           O
ATOM    115  OD2 ASP C 922       2.130 107.378  32.093  1.00 68.31           O
ATOM    116  N   LYS C 923       7.085 108.609  33.559  1.00 67.80           N
ATOM    117  CA  LYS C 923       8.267 107.779  33.713  1.00 66.08           C
ATOM    118  C   LYS C 923       7.884 106.297  33.809  1.00 62.54           C
ATOM    119  O   LYS C 923       8.695 105.440  33.505  1.00 65.36           O
ATOM    120  CB  LYS C 923       9.080 108.228  34.942  1.00 67.57           C
ATOM    121  CG  LYS C 923      10.228 109.196  34.620  1.00 73.58           C
ATOM    122  CD  LYS C 923      11.553 108.468  34.336  1.00 78.66           C
ATOM    123  CE  LYS C 923      12.152 107.810  35.606  1.00 85.47           C
ATOM    124  NZ  LYS C 923      13.465 107.085  35.397  1.00 79.94           N
ATOM    125  N   VAL C 924       6.661 105.978  34.222  1.00 57.97           N
ATOM    126  CA  VAL C 924       6.266 104.569  34.284  1.00 59.25           C
ATOM    127  C   VAL C 924       6.178 103.993  32.855  1.00 60.92           C
ATOM    128  O   VAL C 924       6.643 102.879  32.595  1.00 60.50           O
ATOM    129  CB  VAL C 924       4.903 104.386  35.012  1.00 59.50           C
ATOM    130  CG1 VAL C 924       4.414 102.937  34.899  1.00 51.04           C
ATOM    131  CG2 VAL C 924       5.065 104.748  36.465  1.00 55.92           C
ATOM    132  N   TYR C 925       5.578 104.768  31.947  1.00 59.17           N
ATOM    133  CA  TYR C 925       5.413 104.412  30.538  1.00 58.27           C
ATOM    134  C   TYR C 925       6.798 104.265  29.891  1.00 62.45           C
ATOM    135  O   TYR C 925       7.025 103.397  29.044  1.00 61.60           O
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ATOM    136  CB  TYR C 925       4.613 105.514  29.839  1.00 54.96           C
ATOM    137  CG  TYR C 925       3.947 105.102  28.554  1.00 54.96           C
ATOM    138  CD1 TYR C 925       4.609 105.202  27.336  1.00 58.50           C
ATOM    139  CD2 TYR C 925       2.659 104.582  28.559  1.00 58.34           C
ATOM    140  CE1 TYR C 925       4.003 104.793  26.144  1.00 59.20           C
ATOM    141  CE2 TYR C 925       2.039 104.161  27.376  1.00 58.79           C
ATOM    142  CZ  TYR C 925       2.721 104.270  26.171  1.00 60.73           C
ATOM    143  OH  TYR C 925       2.130 103.849  25.001  1.00 57.74           O
ATOM    144  N   GLU C 926       7.725 105.123  30.299  1.00 65.25           N
ATOM    145  CA  GLU C 926       9.083 105.089  29.780  1.00 68.80           C
ATOM    146  C   GLU C 926       9.809 103.861  30.320  1.00 69.97           C
ATOM    147  O   GLU C 926      10.430 103.099  29.570  1.00 69.90           O
ATOM    148  CB  GLU C 926       9.820 106.358  30.202  1.00 75.59           C
ATOM    149  CG  GLU C 926      11.293 106.408  29.819  1.00 90.96           C
ATOM    150  CD  GLU C 926      11.965 107.723  30.223  1.00101.09           C
ATOM    151  OE1 GLU C 926      11.383 108.464  31.050  1.00109.17           O
ATOM    152  OE2 GLU C 926      13.079 108.010  29.724  1.00106.84           O
ATOM    153  N   ASN C 927       9.717 103.666  31.629  1.00 68.66           N
ATOM    154  CA  ASN C 927      10.376 102.541  32.254  1.00 67.67           C
ATOM    155  C   ASN C 927       9.822 101.200  31.828  1.00 68.74           C
ATOM    156  O   ASN C 927      10.574 100.227  31.768  1.00 72.39           O
ATOM    157  CB  ASN C 927      10.352 102.684  33.773  1.00 68.05           C
ATOM    158  CG  ASN C 927      11.327 103.738  34.259  1.00 70.92           C
ATOM    159  ND2 ASN C 927      11.334 103.976  35.562  1.00 70.63           N
ATOM    160  OD1 ASN C 927      12.072 104.335  33.465  1.00 69.96           O
ATOM    161  N   VAL C 928       8.523 101.126  31.546  1.00 64.92           N
ATOM    162  CA  VAL C 928       7.941  99.868  31.076  1.00 61.66           C
ATOM    163  C   VAL C 928       8.547  99.631  29.700  1.00 60.07           C
ATOM    164  O   VAL C 928       9.082  98.562  29.420  1.00 60.30           O
ATOM    165  CB  VAL C 928       6.392  99.942  30.981  1.00 60.82           C
ATOM    166  CG1 VAL C 928       5.872  98.889  30.022  1.00 60.29           C
ATOM    167  CG2 VAL C 928       5.771  99.725  32.365  1.00 58.20           C
ATOM    168  N   THR C 929       8.485 100.652  28.851  1.00 63.07           N
ATOM    169  CA  THR C 929       9.054 100.578  27.512  1.00 61.40           C
ATOM    170  C   THR C 929      10.504 100.131  27.584  1.00 62.87           C
ATOM    171  O   THR C 929      10.971  99.358  26.749  1.00 63.14           O
ATOM    172  CB  THR C 929       9.003 101.927  26.841  1.00 58.88           C
ATOM    173  CG2 THR C 929       9.757 101.909  25.557  1.00 63.85           C
ATOM    174  OG1 THR C 929       7.646 102.254  26.554  1.00 62.34           O
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ATOM    175  N   GLY C 930      11.216 100.623  28.589  1.00 64.51           N
ATOM    176  CA  GLY C 930      12.602 100.244  28.739  1.00 64.78           C
ATOM    177  C   GLY C 930      12.737  98.768  29.037  1.00 68.72           C
ATOM    178  O   GLY C 930      13.534  98.079  28.411  1.00 73.17           O
ATOM    179  N   LEU C 931      11.958  98.289  30.002  1.00 71.25           N
ATOM    180  CA  LEU C 931      11.973  96.891  30.393  1.00 69.93           C
ATOM    181  C   LEU C 931      11.542  96.037  29.233  1.00 66.95           C
ATOM    182  O   LEU C 931      12.208  95.065  28.914  1.00 67.13           O
ATOM    183  CB  LEU C 931      11.026  96.633  31.565  1.00 73.68           C
ATOM    184  CG  LEU C 931      10.990  95.208  32.125  1.00 77.88           C
ATOM    185  CD1 LEU C 931      12.404  94.755  32.513  1.00 77.15           C
ATOM    186  CD2 LEU C 931      10.054  95.182  33.332  1.00 79.64           C
ATOM    187  N   VAL C 932      10.424  96.365  28.603  1.00 65.09           N
ATOM    188  CA  VAL C 932      10.009  95.537  27.488  1.00 69.46           C
ATOM    189  C   VAL C 932      11.164  95.398  26.517  1.00 73.87           C
ATOM    190  O   VAL C 932      11.497  94.297  26.098  1.00 72.32           O
ATOM    191  CB  VAL C 932       8.820  96.110  26.756  1.00 63.05           C
ATOM    192  CG1 VAL C 932       8.589  95.329  25.483  1.00 62.98           C
ATOM    193  CG2 VAL C 932       7.609  96.025  27.642  1.00 59.58           C
ATOM    194  N   LYS C 933      11.776  96.530  26.185  1.00 79.21           N
ATOM    195  CA  LYS C 933      12.912  96.599  25.274  1.00 80.58           C
ATOM    196  C   LYS C 933      14.141  95.773  25.707  1.00 83.29           C
ATOM    197  O   LYS C 933      14.731  95.054  24.891  1.00 83.49           O
ATOM    198  CB  LYS C 933      13.294  98.064  25.107  1.00 81.60           C
ATOM    199  CG  LYS C 933      13.286  98.550  23.670  1.00 84.45           C
ATOM    200  CD  LYS C 933      12.877 100.009  23.543  1.00 84.61           C
ATOM    201  CE  LYS C 933      11.568 100.112  22.774  1.00 83.57           C
ATOM    202  NZ  LYS C 933      11.236 101.508  22.371  1.00 88.80           N
ATOM    203  N   ALA C 934      14.542  95.872  26.973  1.00 83.91           N
ATOM    204  CA  ALA C 934      15.700  95.101  27.431  1.00 86.68           C
ATOM    205  C   ALA C 934      15.429  93.604  27.294  1.00 88.36           C
ATOM    206  O   ALA C 934      16.351  92.809  27.107  1.00 92.75           O
ATOM    207  CB  ALA C 934      16.048  95.439  28.880  1.00 87.14           C
ATOM    208  N   VAL C 935      14.159  93.227  27.407  1.00 85.45           N
ATOM    209  CA  VAL C 935      13.733  91.839  27.268  1.00 81.49           C
ATOM    210  C   VAL C 935      13.888  91.417  25.814  1.00 81.92           C
ATOM    211  O   VAL C 935      14.375  90.328  25.520  1.00 83.58           O
ATOM    212  CB  VAL C 935      12.247  91.673  27.699  1.00 79.53           C
ATOM    213  CG1 VAL C 935      11.545  90.605  26.852  1.00 72.69           C
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ATOM    214  CG2 VAL C 935      12.184  91.310  29.164  1.00 75.15           C
ATOM    215  N   ILE C 936      13.469  92.291  24.910  1.00 82.93           N
ATOM    216  CA  ILE C 936      13.551  92.020  23.489  1.00 85.97           C
ATOM    217  C   ILE C 936      15.010  91.975  23.021  1.00 92.14           C
ATOM    218  O   ILE C 936      15.336  91.325  22.022  1.00 90.57           O
ATOM    219  CB  ILE C 936      12.766  93.078  22.709  1.00 80.76           C
ATOM    220  CG1 ILE C 936      11.295  93.014  23.104  1.00 78.23           C
ATOM    221  CG2 ILE C 936      12.879  92.827  21.232  1.00 82.49           C
ATOM    222  CD1 ILE C 936      10.444  94.028  22.396  1.00 76.28           C
ATOM    223  N   GLU C 937      15.891  92.658  23.746  1.00 98.38           N
ATOM    224  CA  GLU C 937      17.309  92.662  23.401  1.00105.29           C
ATOM    225  C   GLU C 937      17.875  91.261  23.702  1.00106.70           C
ATOM    226  O   GLU C 937      18.752  90.751  22.996  1.00109.35           O
ATOM    227  CB  GLU C 937      18.034  93.754  24.208  1.00109.34           C
ATOM    228  CG  GLU C 937      19.500  93.990  23.811  1.00114.00           C
ATOM    229  CD  GLU C 937      19.745  93.851  22.306  1.00117.38           C
ATOM    230  OE1 GLU C 937      18.904  94.339  21.512  1.00115.32           O
ATOM    231  OE2 GLU C 937      20.785  93.257  21.925  1.00117.56           O
ATOM    232  N   MET C 938      17.361  90.644  24.761  1.00108.24           N
ATOM    233  CA  MET C 938      17.762  89.296  25.136  1.00107.56           C
ATOM    234  C   MET C 938      16.978  88.301  24.275  1.00108.86           C
ATOM    235  O   MET C 938      17.521  87.303  23.809  1.00107.20           O
ATOM    236  CB  MET C 938      17.444  89.039  26.605  1.00103.15           C
ATOM    237  CG  MET C 938      17.085  87.600  26.890  1.00100.99           C
ATOM    238  SD  MET C 938      16.864  87.280  28.638  1.00102.23           S
ATOM    239  CE  MET C 938      18.424  87.925  29.302  1.00 96.91           C
ATOM    240  N   SER C 939      15.696  88.584  24.061  1.00112.38           N
ATOM    241  CA  SER C 939      14.840  87.692  23.279  1.00117.67           C
ATOM    242  C   SER C 939      15.323  87.446  21.848  1.00119.77           C
ATOM    243  O   SER C 939      15.197  86.328  21.338  1.00118.72           O
ATOM    244  CB  SER C 939      13.392  88.216  23.235  1.00118.43           C
ATOM    245  OG  SER C 939      13.138  88.966  22.054  1.00120.19           O
ATOM    246  N   SER C 940      15.871  88.474  21.200  1.00122.53           N
ATOM    247  CA  SER C 940      16.335  88.328  19.820  1.00124.52           C
ATOM    248  C   SER C 940      17.828  88.067  19.662  1.00125.63           C
ATOM    249  O   SER C 940      18.302  87.764  18.559  1.00123.74           O
ATOM    250  CB  SER C 940      15.955  89.558  19.002  1.00124.34           C
ATOM    251  OG  SER C 940      16.234  89.323  17.633  1.00124.58           O
ATOM    252  N   LYS C 941      18.561  88.199  20.763  1.00127.31           N
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ATOM    253  CA  LYS C 941      19.995  87.954  20.756  1.00130.31           C
ATOM    254  C   LYS C 941      20.260  86.516  21.259  1.00133.31           C
ATOM    255  O   LYS C 941      20.191  85.556  20.483  1.00134.26           O
ATOM    256  CB  LYS C 941      20.706  88.985  21.646  1.00129.68           C
ATOM    257  CG  LYS C 941      22.179  89.203  21.304  1.00133.13           C
ATOM    258  CD  LYS C 941      23.024  87.947  21.534  1.00136.10           C
ATOM    259  CE  LYS C 941      24.242  87.899  20.601  1.00136.33           C
ATOM    260  NZ  LYS C 941      25.034  89.168  20.595  1.00133.87           N
ATOM    261  N   ILE C 942      20.531  86.399  22.563  1.00135.72           N
ATOM    262  CA  ILE C 942      20.832  85.149  23.304  1.00135.88           C
ATOM    263  C   ILE C 942      20.989  83.747  22.671  1.00135.69           C
ATOM    264  O   ILE C 942      21.954  83.048  23.011  1.00136.41           O
ATOM    265  CB  ILE C 942      19.861  84.953  24.508  1.00135.80           C
ATOM    266  CG1 ILE C 942      20.569  84.151  25.618  1.00134.32           C
ATOM    267  CG2 ILE C 942      18.583  84.210  24.062  1.00133.16           C
ATOM    268  CD1 ILE C 942      19.708  83.865  26.818  1.00133.90           C
ATOM    269  N   GLN C 943      20.075  83.315  21.798  1.00134.34           N
ATOM    270  CA  GLN C 943      20.188  81.993  21.193  1.00132.88           C
ATOM    271  C   GLN C 943      21.674  81.652  21.016  1.00132.35           C
ATOM    272  O   GLN C 943      22.173  80.690  21.625  1.00132.00           O
ATOM    273  CB  GLN C 943      19.414  81.962  19.851  1.00132.04           C
ATOM    274  CG  GLN C 943      17.982  81.446  20.006  1.00131.86           C
ATOM    275  CD  GLN C 943      17.936  79.947  20.263  1.00131.58           C
ATOM    276  NE2 GLN C 943      17.400  79.551  21.420  1.00128.52           N
ATOM    277  OE1 GLN C 943      18.384  79.155  19.431  1.00131.63           O
ATOM    278  N   PRO C 944      22.408  82.449  20.194  1.00131.19           N
ATOM    279  CA  PRO C 944      23.835  82.210  19.966  1.00127.40           C
ATOM    280  C   PRO C 944      24.699  82.162  21.238  1.00124.05           C
ATOM    281  O   PRO C 944      25.070  81.116  21.760  1.00122.03           O
ATOM    282  CB  PRO C 944      24.201  83.391  19.093  1.00128.29           C
ATOM    283  CG  PRO C 944      23.087  83.384  18.151  1.00129.04           C
ATOM    284  CD  PRO C 944      21.968  83.466  19.213  1.00130.52           C
ATOM    285  N   ALA C 945      24.992  83.349  21.743  1.00122.53           N
ATOM    286  CA  ALA C 945      25.806  83.568  22.946  1.00122.04           C
ATOM    287  C   ALA C 945      25.841  82.540  24.075  1.00120.54           C
ATOM    288  O   ALA C 945      24.840  81.906  24.400  1.00119.65           O
ATOM    289  CB  ALA C 945      25.494  84.961  23.538  1.00121.84           C
ATOM    290  N   PRO C 946      27.033  82.368  24.685  1.00120.48           N
ATOM    291  CA  PRO C 946      27.308  81.442  25.797  1.00120.10           C
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ATOM    292  C   PRO C 946      27.088  82.176  27.137  1.00118.51           C
ATOM    293  O   PRO C 946      26.599  83.308  27.138  1.00117.33           O
ATOM    294  CB  PRO C 946      28.772  81.055  25.571  1.00121.49           C
ATOM    295  CG  PRO C 946      29.366  82.309  24.986  1.00120.89           C
ATOM    296  CD  PRO C 946      28.288  82.759  24.011  1.00120.40           C
ATOM    297  N   PRO C 947      27.429  81.554  28.284  1.00118.59           N
ATOM    298  CA  PRO C 947      27.252  82.190  29.601  1.00120.40           C
ATOM    299  C   PRO C 947      28.096  83.451  29.875  1.00122.86           C
ATOM    300  O   PRO C 947      27.870  84.150  30.863  1.00121.93           O
ATOM    301  CB  PRO C 947      27.594  81.069  30.570  1.00119.50           C
ATOM    302  CG  PRO C 947      27.130  79.871  29.861  1.00118.56           C
ATOM    303  CD  PRO C 947      27.576  80.097  28.434  1.00118.85           C
ATOM    304  N   GLU C 948      29.105  83.725  29.052  1.00126.09           N
ATOM    305  CA  GLU C 948      29.921  84.935  29.256  1.00128.05           C
ATOM    306  C   GLU C 948      29.179  86.102  28.618  1.00129.22           C
ATOM    307  O   GLU C 948      29.651  87.246  28.633  1.00129.11           O
ATOM    308  CB  GLU C 948      31.281  84.804  28.563  1.00128.79           C
ATOM    309  CG  GLU C 948      32.407  84.236  29.412  1.00129.22           C
ATOM    310  CD  GLU C 948      33.351  83.374  28.595  1.00129.49           C
ATOM    311  OE1 GLU C 948      34.515  83.783  28.369  1.00127.95           O
ATOM    312  OE2 GLU C 948      32.907  82.282  28.171  1.00130.34           O
ATOM    313  N   GLU C 949      27.998  85.811  28.081  1.00130.67           N
ATOM    314  CA  GLU C 949      27.249  86.828  27.372  1.00132.06           C
ATOM    315  C   GLU C 949      25.753  87.036  27.699  1.00131.00           C
ATOM    316  O   GLU C 949      25.239  88.139  27.493  1.00130.08           O
ATOM    317  CB  GLU C 949      27.510  86.591  25.880  1.00134.83           C
ATOM    318  CG  GLU C 949      29.022  86.702  25.559  1.00139.33           C
ATOM    319  CD  GLU C 949      29.411  86.198  24.172  1.00142.36           C
ATOM    320  OE1 GLU C 949      28.784  86.638  23.181  1.00144.45           O
ATOM    321  OE2 GLU C 949      30.356  85.376  24.080  1.00140.95           O
ATOM    322  N   TYR C 950      25.041  86.011  28.181  1.00129.73           N
ATOM    323  CA  TYR C 950      23.648  86.241  28.575  1.00125.37           C
ATOM    324  C   TYR C 950      23.553  86.517  30.088  1.00123.89           C
ATOM    325  O   TYR C 950      22.607  87.168  30.529  1.00124.67           O
ATOM    326  CB  TYR C 950      22.678  85.099  28.172  1.00124.27           C
ATOM    327  CG  TYR C 950      23.065  83.664  28.475  1.00124.30           C
ATOM    328  CD1 TYR C 950      23.439  83.256  29.757  1.00123.25           C
ATOM    329  CD2 TYR C 950      22.993  82.694  27.471  1.00123.52           C
ATOM    330  CE1 TYR C 950      23.729  81.904  30.027  1.00122.44           C
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ATOM    331  CE2 TYR C 950      23.276  81.354  27.728  1.00122.74           C
ATOM    332  CZ  TYR C 950      23.645  80.961  29.000  1.00123.33           C
ATOM    333  OH  TYR C 950      23.933  79.628  29.219  1.00122.73           O
ATOM    334  N   VAL C 951      24.527  86.057  30.879  1.00121.89           N
ATOM    335  CA  VAL C 951      24.483  86.321  32.314  1.00122.76           C
ATOM    336  C   VAL C 951      24.330  87.824  32.567  1.00126.35           C
ATOM    337  O   VAL C 951      23.721  88.226  33.566  1.00128.44           O
ATOM    338  CB  VAL C 951      25.731  85.811  33.041  1.00121.55           C
ATOM    339  CG1 VAL C 951      25.719  86.295  34.493  1.00119.27           C
ATOM    340  CG2 VAL C 951      25.732  84.296  33.010  1.00122.16           C
ATOM    341  N   PRO C 952      24.913  88.677  31.687  1.00127.99           N
ATOM    342  CA  PRO C 952      24.782  90.131  31.868  1.00126.63           C
ATOM    343  C   PRO C 952      23.495  90.571  31.136  1.00125.51           C
ATOM    344  O   PRO C 952      22.759  91.421  31.623  1.00124.87           O
ATOM    345  CB  PRO C 952      26.048  90.694  31.202  1.00126.03           C
ATOM    346  CG  PRO C 952      27.016  89.550  31.238  1.00127.51           C
ATOM    347  CD  PRO C 952      26.122  88.382  30.895  1.00128.76           C
ATOM    348  N   MET C 953      23.236  89.989  29.960  1.00124.90           N
ATOM    349  CA  MET C 953      22.025  90.287  29.161  1.00124.90           C
ATOM    350  C   MET C 953      20.768  90.152  30.033  1.00123.24           C
ATOM    351  O   MET C 953      19.695  90.642  29.674  1.00123.57           O
ATOM    352  CB  MET C 953      21.900  89.307  27.982  1.00128.34           C
ATOM    353  CG  MET C 953      21.893  89.921  26.586  1.00132.89           C
ATOM    354  SD  MET C 953      21.585  88.654  25.299  1.00139.20           S
ATOM    355  CE  MET C 953      23.116  87.639  25.355  1.00133.99           C
ATOM    356  N   VAL C 954      20.914  89.433  31.149  1.00120.10           N
ATOM    357  CA  VAL C 954      19.851  89.218  32.134  1.00115.86           C
ATOM    358  C   VAL C 954      20.044  90.326  33.162  1.00114.76           C
ATOM    359  O   VAL C 954      19.100  91.026  33.523  1.00115.64           O
ATOM    360  CB  VAL C 954      19.980  87.827  32.841  1.00115.37           C
ATOM    361  CG1 VAL C 954      19.528  87.912  34.295  1.00114.62           C
ATOM    362  CG2 VAL C 954      19.132  86.800  32.120  1.00111.15           C
ATOM    363  N   LYS C 955      21.281  90.484  33.625  1.00112.03           N
ATOM    364  CA  LYS C 955      21.611  91.524  34.594  1.00110.08           C
ATOM    365  C   LYS C 955      20.988  92.853  34.129  1.00108.57           C
ATOM    366  O   LYS C 955      20.634  93.707  34.946  1.00107.99           O
ATOM    367  CB  LYS C 955      23.136  91.641  34.715  1.00109.26           C
ATOM    368  CG  LYS C 955      23.618  92.778  35.592  1.00112.85           C
ATOM    369  CD  LYS C 955      23.180  92.635  37.038  1.00113.69           C
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ATOM    370  CE  LYS C 955      23.684  93.818  37.851  1.00117.31           C
ATOM    371  NZ  LYS C 955      23.412  93.674  39.305  1.00120.85           N
ATOM    372  N   GLU C 956      20.849  93.000  32.810  1.00106.12           N
ATOM    373  CA  GLU C 956      20.259  94.183  32.181  1.00104.23           C
ATOM    374  C   GLU C 956      18.766  94.254  32.481  1.00101.34           C
ATOM    375  O   GLU C 956      18.304  95.191  33.132  1.00101.80           O
ATOM    376  CB  GLU C 956      20.462  94.139  30.661  1.00107.40           C
ATOM    377  CG  GLU C 956      21.683  94.881  30.150  1.00115.30           C
ATOM    378  CD  GLU C 956      21.296  96.029  29.238  1.00120.67           C
ATOM    379  OE1 GLU C 956      20.256  95.899  28.554  1.00123.99           O
ATOM    380  OE2 GLU C 956      22.023  97.048  29.192  1.00123.79           O
ATOM    381  N   VAL C 957      18.018  93.275  31.974  1.00 97.84           N
ATOM    382  CA  VAL C 957      16.575  93.179  32.202  1.00 91.30           C
ATOM    383  C   VAL C 957      16.287  93.287  33.705  1.00 89.63           C
ATOM    384  O   VAL C 957      15.201  93.722  34.111  1.00 89.13           O
ATOM    385  CB  VAL C 957      16.024  91.823  31.670  1.00 86.99           C
ATOM    386  CG1 VAL C 957      14.696  91.487  32.325  1.00 81.87           C
ATOM    387  CG2 VAL C 957      15.859  91.885  30.162  1.00 83.49           C
ATOM    388  N   GLY C 958      17.258  92.877  34.521  1.00 86.73           N
ATOM    389  CA  GLY C 958      17.100  92.942  35.963  1.00 86.30           C
ATOM    390  C   GLY C 958      17.253  94.357  36.489  1.00 87.09           C
ATOM    391  O   GLY C 958      16.602  94.736  37.470  1.00 87.61           O
ATOM    392  N   LEU C 959      18.122  95.134  35.836  1.00 88.08           N
ATOM    393  CA  LEU C 959      18.390  96.533  36.203  1.00 87.22           C
ATOM    394  C   LEU C 959      17.248  97.427  35.696  1.00 84.42           C
ATOM    395  O   LEU C 959      16.860  98.399  36.361  1.00 81.73           O
ATOM    396  CB  LEU C 959      19.752  96.998  35.617  1.00 90.23           C
ATOM    397  CG  LEU C 959      21.069  96.402  36.183  1.00 94.61           C
ATOM    398  CD1 LEU C 959      22.235  96.526  35.174  1.00 91.08           C
ATOM    399  CD2 LEU C 959      21.416  97.110  37.493  1.00 96.47           C
ATOM    400  N   ALA C 960      16.710  97.079  34.525  1.00 80.88           N
ATOM    401  CA  ALA C 960      15.614  97.822  33.912  1.00 78.40           C
ATOM    402  C   ALA C 960      14.308  97.632  34.678  1.00 77.74           C
ATOM    403  O   ALA C 960      13.397  98.449  34.574  1.00 77.60           O
ATOM    404  CB  ALA C 960      15.435  97.385  32.474  1.00 77.27           C
ATOM    405  N   LEU C 961      14.216  96.536  35.424  1.00 77.06           N
ATOM    406  CA  LEU C 961      13.037  96.242  36.225  1.00 75.44           C
ATOM    407  C   LEU C 961      13.202  96.911  37.577  1.00 77.45           C
ATOM    408  O   LEU C 961      12.229  97.333  38.204  1.00 76.85           O
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ATOM    409  CB  LEU C 961      12.883  94.737  36.432  1.00 73.48           C
ATOM    410  CG  LEU C 961      11.791  94.360  37.440  1.00 72.22           C
ATOM    411  CD1 LEU C 961      10.410  94.596  36.828  1.00 67.24           C
ATOM    412  CD2 LEU C 961      11.961  92.903  37.858  1.00 73.06           C
ATOM    413  N   ARG C 962      14.440  96.984  38.042  1.00 81.45           N
ATOM    414  CA  ARG C 962      14.714  97.632  39.314  1.00 86.24           C
ATOM    415  C   ARG C 962      14.209  99.069  39.193  1.00 83.35           C
ATOM    416  O   ARG C 962      13.524  99.572  40.085  1.00 83.50           O
ATOM    417  CB  ARG C 962      16.218  97.617  39.594  1.00 96.72           C
ATOM    418  CG  ARG C 962      16.627  98.192  40.952  1.00107.84           C
ATOM    419  CD  ARG C 962      18.157  98.202  41.147  1.00114.40           C
ATOM    420  NE  ARG C 962      18.488  98.556  42.529  1.00123.62           N
ATOM    421  CZ  ARG C 962      19.715  98.810  42.983  1.00127.32           C
ATOM    422  NH1 ARG C 962      20.761  98.751  42.164  1.00129.36           N
ATOM    423  NH2 ARG C 962      19.890  99.139  44.262  1.00127.50           N
ATOM    424  N   THR C 963      14.550  99.700  38.066  1.00 81.04           N
ATOM    425  CA  THR C 963      14.159 101.075  37.737  1.00 77.34           C
ATOM    426  C   THR C 963      12.641 101.222  37.673  1.00 76.41           C
ATOM    427  O   THR C 963      12.077 102.135  38.271  1.00 78.85           O
ATOM    428  CB  THR C 963      14.703 101.532  36.342  1.00 77.75           C
ATOM    429  CG2 THR C 963      14.212 102.939  36.011  1.00 73.04           C
ATOM    430  OG1 THR C 963      16.136 101.527  36.336  1.00 76.39           O
ATOM    431  N   LEU C 964      11.984 100.333  36.931  1.00 72.53           N
ATOM    432  CA  LEU C 964      10.537 100.405  36.784  1.00 71.29           C
ATOM    433  C   LEU C 964       9.855 100.296  38.114  1.00 71.98           C
ATOM    434  O   LEU C 964       8.906 101.030  38.397  1.00 72.44           O
ATOM    435  CB  LEU C 964      10.006  99.298  35.868  1.00 68.42           C
ATOM    436  CG  LEU C 964       8.478  99.135  35.810  1.00 64.26           C
ATOM    437  CD1 LEU C 964       7.791 100.441  35.463  1.00 57.94           C
ATOM    438  CD2 LEU C 964       8.152  98.068  34.782  1.00 62.07           C
ATOM    439  N   LEU C 965      10.341  99.370  38.931  1.00 74.48           N
ATOM    440  CA  LEU C 965       9.764  99.152  40.246  1.00 75.89           C
ATOM    441  C   LEU C 965       9.991 100.384  41.094  1.00 74.88           C
ATOM    442  O   LEU C 965       9.085 100.824  41.815  1.00 73.74           O
ATOM    443  CB  LEU C 965      10.368  97.896  40.879  1.00 76.31           C
ATOM    444  CG  LEU C 965       9.876  96.665  40.106  1.00 76.66           C
ATOM    445  CD1 LEU C 965      10.606  95.443  40.588  1.00 76.56           C
ATOM    446  CD2 LEU C 965       8.357  96.507  40.275  1.00 75.94           C
ATOM    447  N   ALA C 966      11.190 100.954  40.972  1.00 72.90           N
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ATOM    448  CA  ALA C 966      11.550 102.167  41.701  1.00 71.93           C
ATOM    449  C   ALA C 966      10.582 103.315  41.362  1.00 70.46           C
ATOM    450  O   ALA C 966      10.082 103.991  42.268  1.00 72.48           O
ATOM    451  CB  ALA C 966      12.976 102.562  41.371  1.00 69.12           C
ATOM    452  N   THR C 967      10.313 103.520  40.070  1.00 67.44           N
ATOM    453  CA  THR C 967       9.398 104.565  39.627  1.00 63.01           C
ATOM    454  C   THR C 967       7.976 104.304  40.072  1.00 64.40           C
ATOM    455  O   THR C 967       7.271 105.235  40.454  1.00 65.31           O
ATOM    456  CB  THR C 967       9.358 104.693  38.112  1.00 64.08           C
ATOM    457  CG2 THR C 967       8.359 105.741  37.688  1.00 64.42           C
ATOM    458  OG1 THR C 967      10.644 105.078  37.638  1.00 67.54           O
ATOM    459  N   VAL C 968       7.524 103.056  40.012  1.00 63.53           N
ATOM    460  CA  VAL C 968       6.156 102.809  40.440  1.00 65.67           C
ATOM    461  C   VAL C 968       6.079 103.144  41.926  1.00 69.31           C
ATOM    462  O   VAL C 968       5.044 103.603  42.400  1.00 68.50           O
ATOM    463  CB  VAL C 968       5.682 101.338  40.194  1.00 64.11           C
ATOM    464  CG1 VAL C 968       4.207 101.203  40.574  1.00 57.49           C
ATOM    465  CG2 VAL C 968       5.860 100.949  38.731  1.00 60.33           C
ATOM    466  N   ASP C 969       7.181 102.944  42.650  1.00 75.56           N
ATOM    467  CA  ASP C 969       7.206 103.246  44.080  1.00 83.87           C
ATOM    468  C   ASP C 969       7.015 104.739  44.334  1.00 87.31           C
ATOM    469  O   ASP C 969       6.393 105.127  45.328  1.00 90.96           O
ATOM    470  CB  ASP C 969       8.512 102.774  44.730  1.00 90.65           C
ATOM    471  CG  ASP C 969       8.646 101.247  44.743  1.00 99.31           C
ATOM    472  OD1 ASP C 969       7.585 100.569  44.687  1.00 99.15           O
ATOM    473  OD2 ASP C 969       9.804 100.741  44.822  1.00102.67           O
ATOM    474  N   GLU C 970       7.551 105.579  43.451  1.00 87.78           N
ATOM    475  CA  GLU C 970       7.383 107.025  43.592  1.00 87.87           C
ATOM    476  C   GLU C 970       6.020 107.494  43.066  1.00 86.64           C
ATOM    477  O   GLU C 970       5.565 108.587  43.390  1.00 89.18           O
ATOM    478  CB  GLU C 970       8.467 107.757  42.828  1.00 87.52           C
ATOM    479  CG  GLU C 970       9.852 107.398  43.245  1.00 98.17           C
ATOM    480  CD  GLU C 970      10.886 108.142  42.426  1.00107.97           C
ATOM    481  OE1 GLU C 970      10.958 107.886  41.196  1.00110.90           O
ATOM    482  OE2 GLU C 970      11.615 108.980  43.015  1.00110.97           O
ATOM    483  N   THR C 971       5.355 106.657  42.284  1.00 82.40           N
ATOM    484  CA  THR C 971       4.087 107.046  41.711  1.00 79.25           C
ATOM    485  C   THR C 971       2.865 106.634  42.512  1.00 80.67           C
ATOM    486  O   THR C 971       1.841 107.311  42.466  1.00 81.99           O
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ATOM    487  CB  THR C 971       3.993 106.485  40.276  1.00 79.59           C
ATOM    488  CG2 THR C 971       2.685 106.873  39.595  1.00 75.08           C
ATOM    489  OG1 THR C 971       5.091 106.996  39.512  1.00 72.72           O
ATOM    490  N   ILE C 972       2.962 105.531  43.244  1.00 81.67           N
ATOM    491  CA  ILE C 972       1.817 105.045  44.024  1.00 83.42           C
ATOM    492  C   ILE C 972       1.269 106.051  45.048  1.00 80.81           C
ATOM    493  O   ILE C 972       0.046 106.236  45.160  1.00 74.87           O
ATOM    494  CB  ILE C 972       2.166 103.743  44.776  1.00 83.46           C
ATOM    495  CG1 ILE C 972       2.802 102.745  43.820  1.00 84.93           C
ATOM    496  CG2 ILE C 972       0.902 103.090  45.323  1.00 83.58           C
ATOM    497  CD1 ILE C 972       3.825 101.854  44.487  1.00 89.93           C
ATOM    498  N   PRO C 973       2.169 106.709  45.805  1.00 79.99           N
ATOM    499  CA  PRO C 973       1.744 107.687  46.814  1.00 79.69           C
ATOM    500  C   PRO C 973       0.568 108.529  46.339  1.00 80.30           C
ATOM    501  O   PRO C 973      -0.466 108.639  47.004  1.00 81.02           O
ATOM    502  CB  PRO C 973       2.995 108.535  47.016  1.00 76.57           C
ATOM    503  CG  PRO C 973       4.097 107.565  46.802  1.00 75.19           C
ATOM    504  CD  PRO C 973       3.637 106.739  45.625  1.00 76.30           C
ATOM    505  N   LEU C 974       0.765 109.106  45.162  1.00 77.51           N
ATOM    506  CA  LEU C 974      -0.186 109.972  44.493  1.00 75.93           C
ATOM    507  C   LEU C 974      -1.568 109.412  44.101  1.00 74.44           C
ATOM    508  O   LEU C 974      -2.544 110.144  44.073  1.00 75.32           O
ATOM    509  CB  LEU C 974       0.491 110.533  43.243  1.00 76.44           C
ATOM    510  CG  LEU C 974      -0.441 111.137  42.189  1.00 80.68           C
ATOM    511  CD1 LEU C 974      -0.996 112.470  42.673  1.00 80.27           C
ATOM    512  CD2 LEU C 974       0.336 111.310  40.882  1.00 84.93           C
ATOM    513  N   LEU C 975      -1.675 108.129  43.801  1.00 73.62           N
ATOM    514  CA  LEU C 975      -2.967 107.620  43.354  1.00 75.01           C
ATOM    515  C   LEU C 975      -3.926 107.317  44.492  1.00 74.03           C
ATOM    516  O   LEU C 975      -3.518 107.273  45.653  1.00 75.19           O
ATOM    517  CB  LEU C 975      -2.734 106.391  42.475  1.00 75.34           C
ATOM    518  CG  LEU C 975      -1.607 106.735  41.489  1.00 78.17           C
ATOM    519  CD1 LEU C 975      -0.730 105.515  41.226  1.00 79.70           C
ATOM    520  CD2 LEU C 975      -2.208 107.321  40.208  1.00 79.20           C
ATOM    521  N   PRO C 976      -5.222 107.135  44.178  1.00 72.08           N
ATOM    522  CA  PRO C 976      -6.211 106.835  45.216  1.00 74.16           C
ATOM    523  C   PRO C 976      -5.691 105.762  46.154  1.00 75.80           C
ATOM    524  O   PRO C 976      -4.933 104.894  45.741  1.00 79.03           O
ATOM    525  CB  PRO C 976      -7.413 106.388  44.405  1.00 72.85           C
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ATOM    526  CG  PRO C 976      -7.355 107.346  43.252  1.00 69.07           C
ATOM    527  CD  PRO C 976      -5.882 107.359  42.880  1.00 68.30           C
ATOM    528  N   ALA C 977      -6.082 105.823  47.421  1.00 80.66           N
ATOM    529  CA  ALA C 977      -5.611 104.827  48.381  1.00 80.60           C
ATOM    530  C   ALA C 977      -6.081 103.447  47.977  1.00 79.40           C
ATOM    531  O   ALA C 977      -5.274 102.504  47.939  1.00 78.47           O
ATOM    532  CB  ALA C 977      -6.120 105.152  49.803  1.00 79.02           C
ATOM    533  N   SER C 978      -7.378 103.357  47.658  1.00 77.53           N
ATOM    534  CA  SER C 978      -8.031 102.094  47.311  1.00 79.82           C
ATOM    535  C   SER C 978      -7.295 101.299  46.265  1.00 83.07           C
ATOM    536  O   SER C 978      -7.200 100.076  46.359  1.00 88.50           O
ATOM    537  CB  SER C 978      -9.484 102.323  46.851  1.00 77.34           C
ATOM    538  OG  SER C 978      -9.563 102.906  45.566  1.00 79.95           O
ATOM    539  N   THR C 979      -6.742 101.997  45.285  1.00 82.72           N
ATOM    540  CA  THR C 979      -6.036 101.333  44.206  1.00 77.91           C
ATOM    541  C   THR C 979      -4.576 100.906  44.454  1.00 78.02           C
ATOM    542  O   THR C 979      -3.975 100.280  43.582  1.00 79.71           O
ATOM    543  CB  THR C 979      -6.049 102.220  42.970  1.00 74.94           C
ATOM    544  CG2 THR C 979      -7.463 102.693  42.648  1.00 62.47           C
ATOM    545  OG1 THR C 979      -5.230 103.361  43.230  1.00 75.64           O
ATOM    546  N   HIS C 980      -3.995 101.207  45.610  1.00 77.48           N
ATOM    547  CA  HIS C 980      -2.596 100.836  45.805  1.00 79.32           C
ATOM    548  C   HIS C 980      -2.347  99.360  45.884  1.00 78.62           C
ATOM    549  O   HIS C 980      -1.223  98.914  45.667  1.00 76.26           O
ATOM    550  CB  HIS C 980      -2.002 101.472  47.063  1.00 82.98           C
ATOM    551  CG  HIS C 980      -1.892 102.959  46.997  1.00 84.15           C
ATOM    552  CD2 HIS C 980      -2.532 103.867  46.227  1.00 85.49           C
ATOM    553  ND1 HIS C 980      -1.043 103.678  47.815  1.00 85.84           N
ATOM    554  CE1 HIS C 980      -1.170 104.960  47.550  1.00 89.89           C
ATOM    555  NE2 HIS C 980      -2.067 105.111  46.591  1.00 88.60           N
ATOM    556  N   ARG C 981      -3.393  98.604  46.194  1.00 80.21           N
ATOM    557  CA  ARG C 981      -3.273  97.156  46.350  1.00 83.54           C
ATOM    558  C   ARG C 981      -3.079  96.385  45.028  1.00 81.92           C
ATOM    559  O   ARG C 981      -2.167  95.556  44.928  1.00 82.24           O
ATOM    560  CB  ARG C 981      -4.497  96.638  47.135  1.00 85.47           C
ATOM    561  CG  ARG C 981      -4.421  95.184  47.647  1.00 84.60           C
ATOM    562  CD  ARG C 981      -3.350  94.950  48.715  1.00 81.06           C
ATOM    563  NE  ARG C 981      -3.156  93.514  48.938  1.00 83.61           N
ATOM    564  CZ  ARG C 981      -2.444  92.979  49.927  1.00 82.35           C
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ATOM    565  NH1 ARG C 981      -1.841  93.759  50.811  1.00 80.71           N
ATOM    566  NH2 ARG C 981      -2.345  91.657  50.034  1.00 79.63           N
ATOM    567  N   GLU C 982      -3.914  96.656  44.022  1.00 80.43           N
ATOM    568  CA  GLU C 982      -3.786  95.974  42.731  1.00 79.47           C
ATOM    569  C   GLU C 982      -2.404  96.311  42.154  1.00 76.02           C
ATOM    570  O   GLU C 982      -1.742  95.468  41.549  1.00 71.51           O
ATOM    571  CB  GLU C 982      -4.898  96.413  41.748  1.00 80.96           C
ATOM    572  CG  GLU C 982      -5.503  95.242  40.900  1.00 92.71           C
ATOM    573  CD  GLU C 982      -6.581  95.659  39.837  1.00100.52           C
ATOM    574  OE1 GLU C 982      -7.568  96.362  40.206  1.00102.24           O
ATOM    575  OE2 GLU C 982      -6.445  95.262  38.642  1.00 95.96           O
ATOM    576  N   ILE C 983      -1.949  97.532  42.392  1.00 70.78           N
ATOM    577  CA  ILE C 983      -0.664  97.950  41.858  1.00 72.18           C
ATOM    578  C   ILE C 983       0.518  97.342  42.579  1.00 74.15           C
ATOM    579  O   ILE C 983       1.570  97.112  41.982  1.00 77.23           O
ATOM    580  CB  ILE C 983      -0.499  99.493  41.882  1.00 70.97           C
ATOM    581  CG1 ILE C 983      -1.659 100.156  41.129  1.00 66.21           C
ATOM    582  CG2 ILE C 983       0.847  99.874  41.255  1.00 64.06           C
ATOM    583  CD1 ILE C 983      -1.696 101.652  41.230  1.00 60.12           C
ATOM    584  N   GLU C 984       0.365  97.091  43.868  1.00 77.02           N
ATOM    585  CA  GLU C 984       1.468  96.517  44.618  1.00 79.38           C
ATOM    586  C   GLU C 984       1.536  95.055  44.225  1.00 77.09           C
ATOM    587  O   GLU C 984       2.611  94.471  44.090  1.00 74.08           O
ATOM    588  CB  GLU C 984       1.222  96.681  46.119  1.00 88.11           C
ATOM    589  CG  GLU C 984       2.184  97.655  46.801  1.00 99.14           C
ATOM    590  CD  GLU C 984       1.475  98.580  47.793  1.00109.11           C
ATOM    591  OE1 GLU C 984       0.546  98.103  48.497  1.00115.25           O
ATOM    592  OE2 GLU C 984       1.856  99.777  47.871  1.00110.47           O
ATOM    593  N   MET C 985       0.361  94.481  44.016  1.00 73.92           N
ATOM    594  CA  MET C 985       0.245  93.099  43.614  1.00 70.59           C
ATOM    595  C   MET C 985       0.861  92.887  42.213  1.00 69.46           C
ATOM    596  O   MET C 985       1.607  91.926  42.001  1.00 66.72           O
ATOM    597  CB  MET C 985      -1.233  92.703  43.675  1.00 72.71           C
ATOM    598  CG  MET C 985      -1.492  91.613  44.708  1.00 80.42           C
ATOM    599  SD  MET C 985      -0.766  91.853  46.390  1.00 85.30           S
ATOM    600  CE  MET C 985       1.105  91.464  46.198  1.00 82.08           C
ATOM    601  N   ALA C 986       0.546  93.791  41.273  1.00 69.08           N
ATOM    602  CA  ALA C 986       1.086  93.766  39.907  1.00 61.06           C
ATOM    603  C   ALA C 986       2.615  93.820  39.977  1.00 61.60           C
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ATOM    604  O   ALA C 986       3.303  93.201  39.182  1.00 60.41           O
ATOM    605  CB  ALA C 986       0.572  94.944  39.135  1.00 52.88           C
ATOM    606  N   GLN C 987       3.150  94.579  40.923  1.00 64.40           N
ATOM    607  CA  GLN C 987       4.599  94.650  41.083  1.00 69.94           C
ATOM    608  C   GLN C 987       5.205  93.350  41.620  1.00 74.21           C
ATOM    609  O   GLN C 987       6.300  92.942  41.218  1.00 74.81           O
ATOM    610  CB  GLN C 987       4.983  95.727  42.075  1.00 73.29           C
ATOM    611  CG  GLN C 987       4.787  97.131  41.646  1.00 74.46           C
ATOM    612  CD  GLN C 987       5.230  98.082  42.734  1.00 74.15           C
ATOM    613  NE2 GLN C 987       6.511  98.466  42.700  1.00 69.51           N
ATOM    614  OE1 GLN C 987       4.443  98.447  43.616  1.00 71.07           O
ATOM    615  N   LYS C 988       4.530  92.725  42.579  1.00 75.72           N
ATOM    616  CA  LYS C 988       5.067  91.498  43.139  1.00 76.85           C
ATOM    617  C   LYS C 988       5.101  90.456  42.035  1.00 74.61           C
ATOM    618  O   LYS C 988       6.022  89.629  41.960  1.00 75.89           O
ATOM    619  CB  LYS C 988       4.220  91.014  44.326  1.00 83.11           C
ATOM    620  CG  LYS C 988       4.609  89.609  44.824  1.00 93.91           C
ATOM    621  CD  LYS C 988       6.140  89.444  45.039  1.00 98.59           C
ATOM    622  CE  LYS C 988       6.550  87.970  45.192  1.00 96.94           C
ATOM    623  NZ  LYS C 988       7.178  87.683  46.513  1.00101.06           N
ATOM    624  N   LEU C 989       4.100  90.506  41.167  1.00 67.38           N
ATOM    625  CA  LEU C 989       4.039  89.571  40.066  1.00 63.95           C
ATOM    626  C   LEU C 989       5.287  89.710  39.200  1.00 63.62           C
ATOM    627  O   LEU C 989       5.862  88.713  38.787  1.00 63.80           O
ATOM    628  CB  LEU C 989       2.782  89.822  39.246  1.00 60.47           C
ATOM    629  CG  LEU C 989       2.464  88.855  38.113  1.00 57.38           C
ATOM    630  CD1 LEU C 989       2.515  87.434  38.615  1.00 56.34           C
ATOM    631  CD2 LEU C 989       1.091  89.182  37.565  1.00 54.02           C
ATOM    632  N   LEU C 990       5.711  90.940  38.928  1.00 63.58           N
ATOM    633  CA  LEU C 990       6.906  91.159  38.119  1.00 63.56           C
ATOM    634  C   LEU C 990       8.165  90.600  38.784  1.00 64.92           C
ATOM    635  O   LEU C 990       9.055  90.093  38.096  1.00 62.19           O
ATOM    636  CB  LEU C 990       7.084  92.645  37.830  1.00 61.74           C
ATOM    637  CG  LEU C 990       6.074  93.214  36.848  1.00 60.69           C
ATOM    638  CD1 LEU C 990       6.124  94.706  36.887  1.00 60.66           C
ATOM    639  CD2 LEU C 990       6.384  92.706  35.467  1.00 63.00           C
ATOM    640  N   ASN C 991       8.238  90.707  40.111  1.00 67.78           N
ATOM    641  CA  ASN C 991       9.373  90.189  40.880  1.00 73.14           C
ATOM    642  C   ASN C 991       9.567  88.705  40.638  1.00 73.68           C
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ATOM    643  O   ASN C 991      10.670  88.249  40.299  1.00 74.98           O
ATOM    644  CB  ASN C 991       9.158  90.403  42.380  1.00 78.47           C
ATOM    645  CG  ASN C 991       9.744  91.706  42.865  1.00 84.33           C
ATOM    646  ND2 ASN C 991       8.906  92.539  43.479  1.00 87.31           N
ATOM    647  OD1 ASN C 991      10.947  91.965  42.695  1.00 84.79           O
ATOM    648  N   SER C 992       8.486  87.952  40.832  1.00 74.02           N
ATOM    649  CA  SER C 992       8.518  86.516  40.634  1.00 72.44           C
ATOM    650  C   SER C 992       8.788  86.152  39.168  1.00 70.80           C
ATOM    651  O   SER C 992       9.392  85.115  38.911  1.00 71.78           O
ATOM    652  CB  SER C 992       7.216  85.887  41.120  1.00 68.96           C
ATOM    653  OG  SER C 992       6.140  86.325  40.325  1.00 75.27           O
ATOM    654  N   ASP C 993       8.359  86.984  38.213  1.00 71.52           N
ATOM    655  CA  ASP C 993       8.626  86.706  36.793  1.00 72.93           C
ATOM    656  C   ASP C 993      10.134  86.756  36.544  1.00 75.63           C
ATOM    657  O   ASP C 993      10.654  86.008  35.705  1.00 78.90           O
ATOM    658  CB  ASP C 993       7.941  87.725  35.871  1.00 71.56           C
ATOM    659  CG  ASP C 993       6.431  87.555  35.824  1.00 77.47           C
ATOM    660  OD1 ASP C 993       5.900  86.632  36.481  1.00 82.03           O
ATOM    661  OD2 ASP C 993       5.768  88.348  35.125  1.00 81.94           O
ATOM    662  N   LEU C 994      10.823  87.653  37.259  1.00 74.25           N
ATOM    663  CA  LEU C 994      12.268  87.804  37.142  1.00 73.89           C
ATOM    664  C   LEU C 994      12.936  86.630  37.832  1.00 77.39           C
ATOM    665  O   LEU C 994      14.002  86.163  37.408  1.00 77.56           O
ATOM    666  CB  LEU C 994      12.743  89.084  37.805  1.00 73.64           C
ATOM    667  CG  LEU C 994      14.220  89.291  37.510  1.00 71.58           C
ATOM    668  CD1 LEU C 994      14.368  89.691  36.055  1.00 71.16           C
ATOM    669  CD2 LEU C 994      14.777  90.357  38.418  1.00 74.31           C
ATOM    670  N   GLY C 995      12.322  86.184  38.924  1.00 77.11           N
ATOM    671  CA  GLY C 995      12.842  85.034  39.630  1.00 76.87           C
ATOM    672  C   GLY C 995      12.807  83.852  38.671  1.00 76.99           C
ATOM    673  O   GLY C 995      13.779  83.106  38.601  1.00 79.72           O
ATOM    674  N   GLU C 996      11.710  83.681  37.926  1.00 74.12           N
ATOM    675  CA  GLU C 996      11.604  82.574  36.970  1.00 75.44           C
ATOM    676  C   GLU C 996      12.772  82.677  35.997  1.00 75.09           C
ATOM    677  O   GLU C 996      13.544  81.740  35.846  1.00 73.31           O
ATOM    678  CB  GLU C 996      10.274  82.632  36.199  1.00 73.95           C
ATOM    679  CG  GLU C 996       9.818  81.301  35.556  1.00 73.82           C
ATOM    680  CD  GLU C 996       8.433  81.395  34.888  1.00 77.98           C
ATOM    681  OE1 GLU C 996       7.448  81.779  35.563  1.00 75.02           O
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ATOM    682  OE2 GLU C 996       8.325  81.077  33.680  1.00 77.06           O
ATOM    683  N   LEU C 997      12.903  83.835  35.358  1.00 78.06           N
ATOM    684  CA  LEU C 997      13.975  84.087  34.404  1.00 78.32           C
ATOM    685  C   LEU C 997      15.374  83.765  34.937  1.00 78.80           C
ATOM    686  O   LEU C 997      16.201  83.205  34.217  1.00 77.85           O
ATOM    687  CB  LEU C 997      13.936  85.542  33.958  1.00 77.28           C
ATOM    688  CG  LEU C 997      15.135  85.949  33.111  1.00 76.64           C
ATOM    689  CD1 LEU C 997      15.128  85.187  31.794  1.00 73.66           C
ATOM    690  CD2 LEU C 997      15.080  87.437  32.882  1.00 75.03           C
ATOM    691  N   ILE C 998      15.641  84.120  36.189  1.00 77.25           N
ATOM    692  CA  ILE C 998      16.947  83.856  36.778  1.00 80.31           C
ATOM    693  C   ILE C 998      17.186  82.371  37.048  1.00 83.04           C
ATOM    694  O   ILE C 998      18.311  81.881  36.886  1.00 84.10           O
ATOM    695  CB  ILE C 998      17.140  84.687  38.064  1.00 79.40           C
ATOM    696  CG1 ILE C 998      17.338  86.155  37.670  1.00 82.60           C
ATOM    697  CG2 ILE C 998      18.340  84.181  38.859  1.00 77.20           C
ATOM    698  CD1 ILE C 998      16.937  87.149  38.742  1.00 82.48           C
ATOM    699  N   ASN C 999      16.130  81.663  37.448  1.00 83.79           N
ATOM    700  CA  ASN C 999      16.215  80.231  37.715  1.00 80.31           C
ATOM    701  C   ASN C 999      16.506  79.513  36.407  1.00 80.21           C
ATOM    702  O   ASN C 999      17.221  78.514  36.394  1.00 79.90           O
ATOM    703  CB  ASN C 999      14.897  79.681  38.276  1.00 81.63           C
ATOM    704  CG  ASN C 999      14.604  80.160  39.685  1.00 83.96           C
ATOM    705  ND2 ASN C 999      13.329  80.125  40.071  1.00 82.73           N
ATOM    706  OD1 ASN C 999      15.513  80.536  40.426  1.00 87.64           O
ATOM    707  N   LYS C1000      15.939  80.012  35.310  1.00 79.78           N
ATOM    708  CA  LYS C1000      16.156  79.384  34.018  1.00 82.69           C
ATOM    709  C   LYS C1000      17.539  79.701  33.523  1.00 87.29           C
ATOM    710  O   LYS C1000      18.087  78.965  32.713  1.00 91.27           O
ATOM    711  CB  LYS C1000      15.121  79.835  32.986  1.00 81.29           C
ATOM    712  CG  LYS C1000      13.688  79.470  33.362  1.00 83.64           C
ATOM    713  CD  LYS C1000      13.614  78.121  34.082  1.00 82.20           C
ATOM    714  CE  LYS C1000      12.198  77.667  34.392  1.00 78.59           C
ATOM    715  NZ  LYS C1000      12.266  76.569  35.393  1.00 79.19           N
ATOM    716  N   MET C1001      18.111  80.801  34.001  1.00 90.75           N
ATOM    717  CA  MET C1001      19.462  81.159  33.594  1.00 90.87           C
ATOM    718  C   MET C1001      20.436  80.267  34.379  1.00 90.41           C
ATOM    719  O   MET C1001      21.204  79.502  33.786  1.00 86.93           O
ATOM    720  CB  MET C1001      19.746  82.633  33.887  1.00 91.75           C
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ATOM    721  CG  MET C1001      21.171  83.040  33.555  1.00 96.80           C
ATOM    722  SD  MET C1001      21.772  84.462  34.507  1.00104.71           S
ATOM    723  CE  MET C1001      22.116  83.736  36.195  1.00102.20           C
ATOM    724  N   LYS C1002      20.397  80.370  35.709  1.00 87.99           N
ATOM    725  CA  LYS C1002      21.254  79.563  36.573  1.00 89.70           C
ATOM    726  C   LYS C1002      21.318  78.115  36.066  1.00 92.93           C
ATOM    727  O   LYS C1002      22.354  77.457  36.171  1.00 96.73           O
ATOM    728  CB  LYS C1002      20.728  79.572  38.015  1.00 87.91           C
ATOM    729  CG  LYS C1002      21.259  80.674  38.936  1.00 88.01           C
ATOM    730  CD  LYS C1002      20.895  80.339  40.397  1.00 93.03           C
ATOM    731  CE  LYS C1002      21.721  81.109  41.441  1.00 97.29           C
ATOM    732  NZ  LYS C1002      21.562  82.593  41.386  1.00 99.06           N
ATOM    733  N   LEU C1003      20.206  77.622  35.522  1.00 95.37           N
ATOM    734  CA  LEU C1003      20.147  76.259  34.994  1.00 96.66           C
ATOM    735  C   LEU C1003      20.899  76.139  33.678  1.00 98.82           C
ATOM    736  O   LEU C1003      21.751  75.275  33.542  1.00101.68           O
ATOM    737  CB  LEU C1003      18.698  75.791  34.775  1.00 95.97           C
ATOM    738  CG  LEU C1003      17.827  75.312  35.947  1.00 93.54           C
ATOM    739  CD1 LEU C1003      16.393  75.124  35.463  1.00 86.75           C
ATOM    740  CD2 LEU C1003      18.380  74.017  36.524  1.00 89.52           C
ATOM    741  N   ALA C1004      20.595  76.992  32.705  1.00100.95           N
ATOM    742  CA  ALA C1004      21.287  76.907  31.416  1.00103.86           C
ATOM    743  C   ALA C1004      22.817  77.076  31.577  1.00105.77           C
ATOM    744  O   ALA C1004      23.599  76.756  30.667  1.00106.40           O
ATOM    745  CB  ALA C1004      20.717  77.949  30.448  1.00 99.99           C
ATOM    746  N   GLN C1005      23.230  77.565  32.746  1.00104.01           N
ATOM    747  CA  GLN C1005      24.641  77.766  33.051  1.00101.96           C
ATOM    748  C   GLN C1005      25.242  76.479  33.553  1.00101.55           C
ATOM    749  O   GLN C1005      26.385  76.148  33.251  1.00103.75           O
ATOM    750  CB  GLN C1005      24.813  78.829  34.124  1.00101.05           C
ATOM    751  CG  GLN C1005      24.698  80.210  33.593  1.00104.56           C
ATOM    752  CD  GLN C1005      25.625  81.136  34.306  1.00106.03           C
ATOM    753  NE2 GLN C1005      26.756  81.434  33.674  1.00106.95           N
ATOM    754  OE1 GLN C1005      25.346  81.575  35.425  1.00107.39           O
ATOM    755  N   GLN C1006      24.458  75.772  34.349  1.00 98.97           N
ATOM    756  CA  GLN C1006      24.866  74.510  34.917  1.00 96.86           C
ATOM    757  C   GLN C1006      24.851  73.431  33.834  1.00 96.20           C
ATOM    758  O   GLN C1006      25.409  72.350  34.030  1.00 96.22           O
ATOM    759  CB  GLN C1006      23.912  74.172  36.063  1.00 97.68           C
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ATOM    760  CG  GLN C1006      24.048  72.801  36.671  1.00102.93           C
ATOM    761  CD  GLN C1006      23.163  72.647  37.901  1.00107.56           C
ATOM    762  NE2 GLN C1006      23.495  71.685  38.754  1.00109.99           N
ATOM    763  OE1 GLN C1006      22.186  73.382  38.076  1.00110.02           O
ATOM    764  N   TYR C1007      24.228  73.730  32.693  1.00 96.63           N
ATOM    765  CA  TYR C1007      24.142  72.762  31.599  1.00101.98           C
ATOM    766  C   TYR C1007      24.628  73.311  30.265  1.00106.08           C
ATOM    767  O   TYR C1007      23.866  73.388  29.297  1.00105.01           O
ATOM    768  CB  TYR C1007      22.700  72.226  31.454  1.00102.62           C
ATOM    769  CG  TYR C1007      22.205  71.480  32.678  1.00100.68           C
ATOM    770  CD1 TYR C1007      21.822  72.170  33.824  1.00100.14           C
ATOM    771  CD2 TYR C1007      22.223  70.087  32.729  1.00 99.33           C
ATOM    772  CE1 TYR C1007      21.485  71.504  34.990  1.00 98.40           C
ATOM    773  CE2 TYR C1007      21.887  69.408  33.900  1.00 99.82           C
ATOM    774  CZ  TYR C1007      21.521  70.127  35.027  1.00 99.31           C
ATOM    775  OH  TYR C1007      21.209  69.483  36.204  1.00 97.57           O
ATOM    776  N   VAL C1008      25.908  73.689  30.226  1.00112.40           N
ATOM    777  CA  VAL C1008      26.529  74.230  29.009  1.00115.62           C
ATOM    778  C   VAL C1008      27.091  73.120  28.101  1.00118.68           C
ATOM    779  O   VAL C1008      27.695  72.137  28.578  1.00117.20           O
ATOM    780  CB  VAL C1008      27.686  75.220  29.327  1.00113.43           C
ATOM    781  CG1 VAL C1008      27.885  76.188  28.144  1.00111.71           C
ATOM    782  CG2 VAL C1008      27.398  75.965  30.605  1.00110.31           C
ATOM    783  N   MET C1009      26.904  73.311  26.792  1.00119.55           N
ATOM    784  CA  MET C1009      27.340  72.355  25.773  1.00120.49           C
ATOM    785  C   MET C1009      26.614  71.033  26.043  1.00119.74           C
ATOM    786  O   MET C1009      27.248  69.978  26.202  1.00119.45           O
ATOM    787  CB  MET C1009      28.865  72.122  25.825  1.00122.89           C
ATOM    788  CG  MET C1009      29.740  73.355  25.576  1.00121.78           C
ATOM    789  SD  MET C1009      31.003  73.589  26.868  1.00126.30           S
ATOM    790  CE  MET C1009      31.538  71.843  27.253  1.00121.09           C
ATOM    791  N   THR C1010      25.283  71.103  26.109  1.00117.79           N
ATOM    792  CA  THR C1010      24.447  69.925  26.363  1.00112.34           C
ATOM    793  C   THR C1010      23.162  70.041  25.546  1.00109.06           C
ATOM    794  O   THR C1010      22.902  71.063  24.904  1.00107.42           O
ATOM    795  CB  THR C1010      24.040  69.810  27.873  1.00110.10           C
ATOM    796  CG2 THR C1010      23.531  68.420  28.191  1.00110.33           C
ATOM    797  OG1 THR C1010      25.175  70.047  28.712  1.00105.49           O
ATOM    798  N   SER C1011      22.369  68.980  25.563  1.00106.23           N
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ATOM    799  CA  SER C1011      21.088  68.985  24.876  1.00106.87           C
ATOM    800  C   SER C1011      20.139  69.820  25.756  1.00107.19           C
ATOM    801  O   SER C1011      19.082  70.297  25.308  1.00102.61           O
ATOM    802  CB  SER C1011      20.578  67.549  24.762  1.00107.83           C
ATOM    803  OG  SER C1011      20.787  66.826  25.974  1.00104.56           O
ATOM    804  N   LEU C1012      20.543  69.982  27.020  1.00107.60           N
ATOM    805  CA  LEU C1012      19.753  70.719  28.003  1.00107.90           C
ATOM    806  C   LEU C1012      19.973  72.207  27.945  1.00109.30           C
ATOM    807  O   LEU C1012      19.075  72.984  28.287  1.00110.31           O
ATOM    808  CB  LEU C1012      20.015  70.220  29.438  1.00104.23           C
ATOM    809  CG  LEU C1012      19.319  68.895  29.812  1.00103.41           C
ATOM    810  CD1 LEU C1012      19.096  68.867  31.327  1.00 99.74           C
ATOM    811  CD2 LEU C1012      17.969  68.739  29.062  1.00 97.65           C
ATOM    812  N   GLN C1013      21.164  72.600  27.505  1.00110.00           N
ATOM    813  CA  GLN C1013      21.506  74.009  27.394  1.00108.04           C
ATOM    814  C   GLN C1013      20.532  74.741  26.469  1.00104.48           C
ATOM    815  O   GLN C1013      20.138  75.874  26.739  1.00103.94           O
ATOM    816  CB  GLN C1013      22.928  74.158  26.862  1.00110.51           C
ATOM    817  CG  GLN C1013      23.373  75.603  26.716  1.00113.77           C
ATOM    818  CD  GLN C1013      24.452  75.747  25.670  1.00113.99           C
ATOM    819  NE2 GLN C1013      24.084  76.308  24.522  1.00112.15           N
ATOM    820  OE1 GLN C1013      25.600  75.339  25.876  1.00113.81           O
ATOM    821  N   GLN C1014      20.157  74.098  25.371  1.00102.14           N
ATOM    822  CA  GLN C1014      19.235  74.718  24.440  1.00100.91           C
ATOM    823  C   GLN C1014      17.838  74.778  25.043  1.00102.05           C
ATOM    824  O   GLN C1014      17.068  75.682  24.723  1.00104.42           O
ATOM    825  CB  GLN C1014      19.194  73.944  23.119  1.00102.30           C
ATOM    826  CG  GLN C1014      18.388  74.634  22.009  1.00110.82           C
ATOM    827  CD  GLN C1014      16.952  74.110  21.851  1.00115.56           C
ATOM    828  NE2 GLN C1014      16.046  74.585  22.709  1.00115.52           N
ATOM    829  OE1 GLN C1014      16.667  73.288  20.966  1.00116.95           O
ATOM    830  N   GLU C1015      17.510  73.830  25.926  1.00100.51           N
ATOM    831  CA  GLU C1015      16.178  73.788  26.534  1.00 95.53           C
ATOM    832  C   GLU C1015      15.959  74.945  27.489  1.00 90.60           C
ATOM    833  O   GLU C1015      15.087  75.788  27.249  1.00 84.83           O
ATOM    834  CB  GLU C1015      15.948  72.449  27.250  1.00 97.24           C
ATOM    835  CG  GLU C1015      14.516  72.235  27.763  1.00101.85           C
ATOM    836  CD  GLU C1015      13.407  72.502  26.710  1.00104.25           C
ATOM    837  OE1 GLU C1015      13.570  72.137  25.521  1.00100.17           O
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ATOM    838  OE2 GLU C1015      12.350  73.065  27.091  1.00103.74           O
ATOM    839  N   TYR C1016      16.768  74.996  28.544  1.00 86.99           N
ATOM    840  CA  TYR C1016      16.673  76.060  29.532  1.00 90.23           C
ATOM    841  C   TYR C1016      16.819  77.464  28.935  1.00 91.23           C
ATOM    842  O   TYR C1016      16.740  78.461  29.666  1.00 91.81           O
ATOM    843  CB  TYR C1016      17.702  75.847  30.649  1.00 92.03           C
ATOM    844  CG  TYR C1016      17.413  74.621  31.485  1.00 96.31           C
ATOM    845  CD1 TYR C1016      16.145  74.410  32.027  1.00 95.33           C
ATOM    846  CD2 TYR C1016      18.383  73.639  31.681  1.00 99.21           C
ATOM    847  CE1 TYR C1016      15.844  73.247  32.736  1.00 97.48           C
ATOM    848  CE2 TYR C1016      18.090  72.467  32.394  1.00 98.50           C
ATOM    849  CZ  TYR C1016      16.817  72.282  32.915  1.00 96.64           C
ATOM    850  OH  TYR C1016      16.513  71.138  33.617  1.00 95.40           O
ATOM    851  N   LYS C1017      17.041  77.543  27.622  1.00 90.88           N
ATOM    852  CA  LYS C1017      17.140  78.835  26.949  1.00 89.24           C
ATOM    853  C   LYS C1017      15.755  79.157  26.417  1.00 85.90           C
ATOM    854  O   LYS C1017      15.328  80.314  26.415  1.00 82.40           O
ATOM    855  CB  LYS C1017      18.142  78.810  25.787  1.00 93.74           C
ATOM    856  CG  LYS C1017      19.596  79.054  26.190  1.00 96.49           C
ATOM    857  CD  LYS C1017      20.433  79.517  24.996  1.00 96.88           C
ATOM    858  CE  LYS C1017      21.907  79.641  25.351  1.00 98.92           C
ATOM    859  NZ  LYS C1017      22.677  80.119  24.171  1.00100.42           N
ATOM    860  N   LYS C1018      15.055  78.131  25.949  1.00 83.14           N
ATOM    861  CA  LYS C1018      13.708  78.342  25.457  1.00 87.47           C
ATOM    862  C   LYS C1018      12.835  78.752  26.640  1.00 87.65           C
ATOM    863  O   LYS C1018      11.830  79.466  26.483  1.00 84.27           O
ATOM    864  CB  LYS C1018      13.169  77.070  24.822  1.00 89.97           C
ATOM    865  CG  LYS C1018      13.613  76.895  23.399  1.00 96.20           C
ATOM    866  CD  LYS C1018      12.885  75.739  22.745  1.00103.28           C
ATOM    867  CE  LYS C1018      13.303  75.560  21.291  1.00104.51           C
ATOM    868  NZ  LYS C1018      12.940  74.192  20.792  1.00103.98           N
ATOM    869  N   GLN C1019      13.241  78.285  27.822  1.00 85.24           N
ATOM    870  CA  GLN C1019      12.546  78.585  29.061  1.00 80.75           C
ATOM    871  C   GLN C1019      12.922  79.979  29.522  1.00 82.79           C
ATOM    872  O   GLN C1019      12.105  80.666  30.135  1.00 86.11           O
ATOM    873  CB  GLN C1019      12.873  77.535  30.125  1.00 74.33           C
ATOM    874  CG  GLN C1019      12.050  76.272  29.950  1.00 72.25           C
ATOM    875  CD  GLN C1019      12.450  75.178  30.917  1.00 73.41           C
ATOM    876  NE2 GLN C1019      12.486  73.935  30.434  1.00 77.00           N
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ATOM    877  OE1 GLN C1019      12.715  75.442  32.088  1.00 72.63           O
ATOM    878  N   MET C1020      14.154  80.399  29.236  1.00 85.11           N
ATOM    879  CA  MET C1020      14.577  81.749  29.591  1.00 84.66           C
ATOM    880  C   MET C1020      13.717  82.684  28.746  1.00 83.25           C
ATOM    881  O   MET C1020      13.164  83.656  29.247  1.00 83.62           O
ATOM    882  CB  MET C1020      16.067  81.966  29.285  1.00 85.31           C
ATOM    883  CG  MET C1020      16.959  81.858  30.524  1.00 90.41           C
ATOM    884  SD  MET C1020      18.753  81.804  30.222  1.00 91.63           S
ATOM    885  CE  MET C1020      19.239  83.527  30.360  1.00 88.91           C
ATOM    886  N   LEU C1021      13.587  82.377  27.462  1.00 80.01           N
ATOM    887  CA  LEU C1021      12.779  83.218  26.596  1.00 81.04           C
ATOM    888  C   LEU C1021      11.353  83.338  27.097  1.00 81.68           C
ATOM    889  O   LEU C1021      10.759  84.411  27.065  1.00 80.93           O
ATOM    890  CB  LEU C1021      12.737  82.661  25.179  1.00 84.04           C
ATOM    891  CG  LEU C1021      13.983  82.688  24.301  1.00 83.49           C
ATOM    892  CD1 LEU C1021      13.507  83.028  22.895  1.00 80.96           C
ATOM    893  CD2 LEU C1021      14.998  83.724  24.779  1.00 80.98           C
ATOM    894  N   THR C1022      10.811  82.207  27.531  1.00 84.90           N
ATOM    895  CA  THR C1022       9.446  82.110  28.037  1.00 85.69           C
ATOM    896  C   THR C1022       9.251  83.048  29.208  1.00 83.51           C
ATOM    897  O   THR C1022       8.390  83.934  29.197  1.00 80.07           O
ATOM    898  CB  THR C1022       9.154  80.637  28.469  1.00 88.46           C
ATOM    899  CG2 THR C1022       8.259  80.570  29.712  1.00 90.20           C
ATOM    900  OG1 THR C1022       8.543  79.941  27.374  1.00 91.00           O
ATOM    901  N   ALA C1023      10.092  82.826  30.208  1.00 81.70           N
ATOM    902  CA  ALA C1023      10.094  83.586  31.436  1.00 83.77           C
ATOM    903  C   ALA C1023      10.250  85.077  31.213  1.00 85.16           C
ATOM    904  O   ALA C1023       9.714  85.859  31.998  1.00 89.04           O
ATOM    905  CB  ALA C1023      11.210  83.085  32.352  1.00 83.59           C
ATOM    906  N   ALA C1024      10.980  85.470  30.163  1.00 81.68           N
ATOM    907  CA  ALA C1024      11.214  86.887  29.875  1.00 75.41           C
ATOM    908  C   ALA C1024      10.025  87.513  29.145  1.00 73.27           C
ATOM    909  O   ALA C1024       9.701  88.680  29.359  1.00 72.93           O
ATOM    910  CB  ALA C1024      12.501  87.061  29.070  1.00 65.77           C
ATOM    911  N   HIS C1025       9.369  86.740  28.290  1.00 68.05           N
ATOM    912  CA  HIS C1025       8.209  87.249  27.576  1.00 68.21           C
ATOM    913  C   HIS C1025       7.117  87.527  28.621  1.00 69.52           C
ATOM    914  O   HIS C1025       6.305  88.444  28.459  1.00 65.51           O
ATOM    915  CB  HIS C1025       7.727  86.206  26.551  1.00 71.98           C
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ATOM    916  CG  HIS C1025       6.534  86.631  25.743  1.00 78.78           C
ATOM    917  CD2 HIS C1025       6.449  87.173  24.501  1.00 83.90           C
ATOM    918  ND1 HIS C1025       5.237  86.520  26.198  1.00 84.22           N
ATOM    919  CE1 HIS C1025       4.406  86.975  25.277  1.00 87.90           C
ATOM    920  NE2 HIS C1025       5.113  87.378  24.237  1.00 86.95           N
ATOM    921  N   ALA C1026       7.119  86.732  29.696  1.00 68.89           N
ATOM    922  CA  ALA C1026       6.127  86.843  30.766  1.00 66.22           C
ATOM    923  C   ALA C1026       6.342  88.146  31.470  1.00 67.21           C
ATOM    924  O   ALA C1026       5.411  88.917  31.693  1.00 70.82           O
ATOM    925  CB  ALA C1026       6.289  85.720  31.729  1.00 59.99           C
ATOM    926  N   LEU C1027       7.594  88.373  31.826  1.00 65.47           N
ATOM    927  CA  LEU C1027       7.994  89.597  32.467  1.00 63.68           C
ATOM    928  C   LEU C1027       7.507  90.779  31.624  1.00 64.67           C
ATOM    929  O   LEU C1027       7.048  91.774  32.164  1.00 70.41           O
ATOM    930  CB  LEU C1027       9.516  89.625  32.591  1.00 60.17           C
ATOM    931  CG  LEU C1027      10.140  90.845  33.254  1.00 61.80           C
ATOM    932  CD1 LEU C1027       9.381  91.159  34.512  1.00 64.53           C
ATOM    933  CD2 LEU C1027      11.599  90.582  33.579  1.00 66.87           C
ATOM    934  N   ALA C1028       7.577  90.669  30.302  1.00 62.81           N
ATOM    935  CA  ALA C1028       7.152  91.773  29.448  1.00 63.80           C
ATOM    936  C   ALA C1028       5.645  91.975  29.356  1.00 64.53           C
ATOM    937  O   ALA C1028       5.173  93.107  29.348  1.00 63.07           O
ATOM    938  CB  ALA C1028       7.717  91.600  28.068  1.00 62.94           C
ATOM    939  N   VAL C1029       4.890  90.887  29.265  1.00 66.59           N
ATOM    940  CA  VAL C1029       3.439  90.986  29.172  1.00 67.48           C
ATOM    941  C   VAL C1029       2.884  91.582  30.461  1.00 67.97           C
ATOM    942  O   VAL C1029       1.915  92.351  30.448  1.00 65.88           O
ATOM    943  CB  VAL C1029       2.824  89.607  28.930  1.00 66.88           C
ATOM    944  CG1 VAL C1029       1.330  89.730  28.727  1.00 63.81           C
ATOM    945  CG2 VAL C1029       3.472  88.985  27.709  1.00 66.42           C
ATOM    946  N   ASP C1030       3.521  91.222  31.570  1.00 65.23           N
ATOM    947  CA  ASP C1030       3.126  91.712  32.880  1.00 64.94           C
ATOM    948  C   ASP C1030       3.488  93.173  33.094  1.00 62.44           C
ATOM    949  O   ASP C1030       2.701  93.927  33.658  1.00 64.35           O
ATOM    950  CB  ASP C1030       3.735  90.839  33.992  1.00 65.96           C
ATOM    951  CG  ASP C1030       2.911  89.578  34.255  1.00 69.57           C
ATOM    952  OD1 ASP C1030       1.701  89.591  33.944  1.00 67.28           O
ATOM    953  OD2 ASP C1030       3.454  88.585  34.783  1.00 71.94           O
ATOM    954  N   ALA C1031       4.668  93.576  32.643  1.00 59.88           N
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ATOM    955  CA  ALA C1031       5.072  94.959  32.796  1.00 57.53           C
ATOM    956  C   ALA C1031       4.022  95.837  32.109  1.00 59.49           C
ATOM    957  O   ALA C1031       3.706  96.935  32.579  1.00 58.64           O
ATOM    958  CB  ALA C1031       6.428  95.162  32.176  1.00 51.37           C
ATOM    959  N   LYS C1032       3.470  95.345  31.002  1.00 59.00           N
ATOM    960  CA  LYS C1032       2.466  96.094  30.270  1.00 57.05           C
ATOM    961  C   LYS C1032       1.148  96.057  31.023  1.00 60.38           C
ATOM    962  O   LYS C1032       0.296  96.936  30.854  1.00 57.03           O
ATOM    963  CB  LYS C1032       2.309  95.513  28.862  1.00 56.79           C
ATOM    964  CG  LYS C1032       3.458  95.897  27.918  1.00 62.37           C
ATOM    965  CD  LYS C1032       3.612  94.970  26.703  1.00 68.50           C
ATOM    966  CE  LYS C1032       2.945  95.535  25.447  1.00 72.18           C
ATOM    967  NZ  LYS C1032       3.085  94.605  24.287  1.00 75.66           N
ATOM    968  N   ASN C1033       0.971  95.031  31.855  1.00 63.06           N
ATOM    969  CA  ASN C1033      -0.264  94.919  32.623  1.00 62.59           C
ATOM    970  C   ASN C1033      -0.163  95.835  33.817  1.00 59.41           C
ATOM    971  O   ASN C1033      -1.151  96.441  34.210  1.00 57.40           O
ATOM    972  CB  ASN C1033      -0.530  93.471  33.044  1.00 64.82           C
ATOM    973  CG  ASN C1033      -1.004  92.614  31.880  1.00 74.38           C
ATOM    974  ND2 ASN C1033      -1.214  93.253  30.728  1.00 79.97           N
ATOM    975  OD1 ASN C1033      -1.185  91.398  32.009  1.00 78.02           O
ATOM    976  N   LEU C1034       1.039  95.945  34.375  1.00 56.92           N
ATOM    977  CA  LEU C1034       1.276  96.829  35.495  1.00 55.84           C
ATOM    978  C   LEU C1034       0.805  98.193  35.032  1.00 59.67           C
ATOM    979  O   LEU C1034      -0.033  98.835  35.671  1.00 65.25           O
ATOM    980  CB  LEU C1034       2.760  96.887  35.807  1.00 56.08           C
ATOM    981  CG  LEU C1034       3.112  97.924  36.866  1.00 64.48           C
ATOM    982  CD1 LEU C1034       2.306  97.609  38.101  1.00 67.21           C
ATOM    983  CD2 LEU C1034       4.603  97.907  37.181  1.00 64.72           C
ATOM    984  N   LEU C1035       1.357  98.626  33.903  1.00 58.09           N
ATOM    985  CA  LEU C1035       1.020  99.901  33.296  1.00 55.87           C
ATOM    986  C   LEU C1035      -0.486 100.027  33.167  1.00 51.30           C
ATOM    987  O   LEU C1035      -1.049 101.029  33.547  1.00 48.73           O
ATOM    988  CB  LEU C1035       1.658  99.996  31.916  1.00 58.28           C
ATOM    989  CG  LEU C1035       1.914 101.349  31.273  1.00 59.39           C
ATOM    990  CD1 LEU C1035       2.086 101.110  29.799  1.00 59.31           C
ATOM    991  CD2 LEU C1035       0.767 102.299  31.500  1.00 62.27           C
ATOM    992  N   ASP C1036      -1.143  99.014  32.622  1.00 53.83           N
ATOM    993  CA  ASP C1036      -2.592  99.079  32.488  1.00 58.81           C
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ATOM    994  C   ASP C1036      -3.343  99.361  33.809  1.00 60.83           C
ATOM    995  O   ASP C1036      -4.246 100.197  33.825  1.00 58.01           O
ATOM    996  CB  ASP C1036      -3.127  97.802  31.862  1.00 63.90           C
ATOM    997  CG  ASP C1036      -4.650  97.795  31.771  1.00 75.23           C
ATOM    998  OD1 ASP C1036      -5.274  96.953  32.452  1.00 86.78           O
ATOM    999  OD2 ASP C1036      -5.224  98.627  31.032  1.00 80.05           O
ATOM   1000  N   VAL C1037      -2.998  98.656  34.892  1.00 63.64           N
ATOM   1001  CA  VAL C1037      -3.616  98.860  36.209  1.00 63.82           C
ATOM   1002  C   VAL C1037      -3.492 100.351  36.588  1.00 65.23           C
ATOM   1003  O   VAL C1037      -4.497 101.060  36.788  1.00 68.35           O
ATOM   1004  CB  VAL C1037      -2.887  98.017  37.278  1.00 65.81           C
ATOM   1005  CG1 VAL C1037      -3.460  98.265  38.655  1.00 63.68           C
ATOM   1006  CG2 VAL C1037      -3.008  96.576  36.932  1.00 66.00           C
ATOM   1007  N   ILE C1038      -2.254 100.830  36.684  1.00 56.67           N
ATOM   1008  CA  ILE C1038      -1.988 102.232  37.008  1.00 52.09           C
ATOM   1009  C   ILE C1038      -2.795 103.253  36.154  1.00 56.52           C
ATOM   1010  O   ILE C1038      -3.207 104.319  36.643  1.00 61.00           O
ATOM   1011  CB  ILE C1038      -0.506 102.495  36.857  1.00 40.92           C
ATOM   1012  CG1 ILE C1038       0.251 101.813  37.991  1.00 40.83           C
ATOM   1013  CG2 ILE C1038      -0.241 103.944  36.878  1.00 44.37           C
ATOM   1014  CD1 ILE C1038       1.781 101.856  37.871  1.00 43.08           C
ATOM   1015  N   ASP C1039      -3.016 102.951  34.880  1.00 58.87           N
ATOM   1016  CA  ASP C1039      -3.788 103.863  34.044  1.00 63.24           C
ATOM   1017  C   ASP C1039      -5.223 103.847  34.553  1.00 62.31           C
ATOM   1018  O   ASP C1039      -5.846 104.903  34.639  1.00 61.21           O
ATOM   1019  CB  ASP C1039      -3.712 103.478  32.540  1.00 64.64           C
ATOM   1020  CG  ASP C1039      -2.406 103.983  31.850  1.00 70.50           C
ATOM   1021  OD1 ASP C1039      -1.519 104.598  32.524  1.00 64.94           O
ATOM   1022  OD2 ASP C1039      -2.283 103.749  30.621  1.00 73.26           O
ATOM   1023  N   GLN C1040      -5.755 102.667  34.885  1.00 63.31           N
ATOM   1024  CA  GLN C1040      -7.122 102.585  35.423  1.00 66.22           C
ATOM   1025  C   GLN C1040      -7.111 103.430  36.720  1.00 65.53           C
ATOM   1026  O   GLN C1040      -8.056 104.175  37.036  1.00 57.11           O
ATOM   1027  CB  GLN C1040      -7.481 101.143  35.783  1.00 69.30           C
ATOM   1028  CG  GLN C1040      -7.457 100.156  34.667  1.00 80.10           C
ATOM   1029  CD  GLN C1040      -7.681  98.738  35.175  1.00 87.83           C
ATOM   1030  NE2 GLN C1040      -6.715  97.844  34.925  1.00 91.51           N
ATOM   1031  OE1 GLN C1040      -8.711  98.452  35.790  1.00 91.10           O
ATOM   1032  N   ALA C1041      -6.022 103.283  37.469  1.00 62.66           N
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ATOM   1033  CA  ALA C1041      -5.853 104.025  38.698  1.00 62.47           C
ATOM   1034  C   ALA C1041      -5.868 105.525  38.400  1.00 66.44           C
ATOM   1035  O   ALA C1041      -6.569 106.275  39.088  1.00 69.97           O
ATOM   1036  CB  ALA C1041      -4.539 103.635  39.384  1.00 59.49           C
ATOM   1037  N   ARG C1042      -5.125 105.994  37.398  1.00 65.45           N
ATOM   1038  CA  ARG C1042      -5.170 107.435  37.161  1.00 67.91           C
ATOM   1039  C   ARG C1042      -6.545 107.875  36.667  1.00 68.21           C
ATOM   1040  O   ARG C1042      -7.045 108.920  37.077  1.00 67.77           O
ATOM   1041  CB  ARG C1042      -4.091 107.883  36.179  1.00 63.15           C
ATOM   1042  CG  ARG C1042      -2.707 107.699  36.725  1.00 64.59           C
ATOM   1043  CD  ARG C1042      -1.821 107.089  35.661  1.00 64.74           C
ATOM   1044  NE  ARG C1042      -0.396 107.291  35.918  1.00 58.12           N
ATOM   1045  CZ  ARG C1042       0.562 107.019  35.038  1.00 55.70           C
ATOM   1046  NH1 ARG C1042       0.252 106.537  33.842  1.00 57.33           N
ATOM   1047  NH2 ARG C1042       1.829 107.216  35.350  1.00 49.95           N
ATOM   1048  N   LEU C1043      -7.161 107.079  35.801  1.00 68.03           N
ATOM   1049  CA  LEU C1043      -8.468 107.436  35.285  1.00 73.06           C
ATOM   1050  C   LEU C1043      -9.472 107.546  36.432  1.00 78.30           C
ATOM   1051  O   LEU C1043     -10.299 108.463  36.451  1.00 77.88           O
ATOM   1052  CB  LEU C1043      -8.927 106.404  34.246  1.00 69.68           C
ATOM   1053  CG  LEU C1043      -8.057 106.338  32.978  1.00 69.22           C
ATOM   1054  CD1 LEU C1043      -8.528 105.195  32.108  1.00 66.15           C
ATOM   1055  CD2 LEU C1043      -8.101 107.653  32.205  1.00 62.85           C
ATOM   1056  N   LYS C1044      -9.389 106.622  37.393  1.00 83.18           N
ATOM   1057  CA  LYS C1044     -10.296 106.640  38.539  1.00 84.86           C
ATOM   1058  C   LYS C1044     -10.144 107.999  39.194  1.00 85.31           C
ATOM   1059  O   LYS C1044     -11.079 108.803  39.239  1.00 85.59           O
ATOM   1060  CB  LYS C1044      -9.934 105.558  39.566  1.00 85.94           C
ATOM   1061  CG  LYS C1044     -11.166 104.960  40.237  1.00 91.52           C
ATOM   1062  CD  LYS C1044     -10.911 104.331  41.601  1.00 91.04           C
ATOM   1063  CE  LYS C1044     -12.193 103.660  42.097  1.00 90.64           C
ATOM   1064  NZ  LYS C1044     -12.051 103.064  43.449  1.00 91.14           N
ATOM   1065  N   MET C1045      -8.939 108.256  39.681  1.00 82.94           N
ATOM   1066  CA  MET C1045      -8.640 109.505  40.346  1.00 82.97           C
ATOM   1067  C   MET C1045      -9.061 110.743  39.567  1.00 87.45           C
ATOM   1068  O   MET C1045      -9.165 111.818  40.147  1.00 92.61           O
ATOM   1069  CB  MET C1045      -7.155 109.588  40.649  1.00 79.19           C
ATOM   1070  CG  MET C1045      -6.747 110.838  41.370  1.00 77.81           C
ATOM   1071  SD  MET C1045      -4.965 110.819  41.573  1.00 91.61           S
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ATOM   1072  CE  MET C1045      -4.779 112.247  42.618  1.00 93.10           C
ATOM   1073  N   LEU C1046      -9.283 110.618  38.261  1.00 89.77           N
ATOM   1074  CA  LEU C1046      -9.693 111.779  37.467  1.00 92.15           C
ATOM   1075  C   LEU C1046     -11.217 111.928  37.380  1.00 94.43           C
ATOM   1076  O   LEU C1046     -11.732 113.043  37.230  1.00 93.71           O
ATOM   1077  CB  LEU C1046      -9.086 111.717  36.056  1.00 88.87           C
ATOM   1078  CG  LEU C1046      -7.660 112.254  35.905  1.00 87.24           C
ATOM   1079  CD1 LEU C1046      -7.175 112.075  34.478  1.00 85.35           C
ATOM   1080  CD2 LEU C1046      -7.641 113.718  36.283  1.00 85.90           C
ATOM   1081  N   GLY C1047     -11.923 110.801  37.483  1.00 96.12           N
ATOM   1082  CA  GLY C1047     -13.378 110.801  37.433  1.00102.00           C
ATOM   1083  C   GLY C1047     -14.033 110.519  38.786  1.00106.82           C
ATOM   1084  O   GLY C1047     -14.645 109.431  38.946  1.00108.43           O
TER    1085      GLY C1047
ATOM   1055  N   THR D   2       1.264 104.168  23.824  1.00117.75           N
ATOM   1056  CA  THR D   2       1.121 102.693  23.972  1.00119.14           C
ATOM   1057  C   THR D   2       0.948 102.019  22.616  1.00120.27           C
ATOM   1058  O   THR D   2       0.822 100.802  22.543  1.00120.61           O
ATOM   1059  CB  THR D   2      -0.072 102.329  24.931  1.00119.19           C
ATOM   1060  CG2 THR D   2      -0.381 100.832  24.916  1.00114.83           C
ATOM   1061  OG1 THR D   2       0.278 102.693  26.273  1.00119.79           O
ATOM   1062  N   ARG D   3       0.943 102.794  21.534  1.00122.00           N
ATOM   1063  CA  ARG D   3       0.821 102.183  20.212  1.00122.43           C
ATOM   1064  C   ARG D   3       2.247 101.762  19.825  1.00121.24           C
ATOM   1065  O   ARG D   3       2.438 100.766  19.122  1.00120.23           O
ATOM   1066  CB  ARG D   3       0.221 103.170  19.188  1.00124.89           C
ATOM   1067  CG  ARG D   3      -0.729 102.504  18.181  1.00127.61           C
ATOM   1068  CD  ARG D   3      -1.341 103.504  17.189  1.00131.95           C
ATOM   1069  NE  ARG D   3      -2.370 104.358  17.787  1.00136.27           N
ATOM   1070  CZ  ARG D   3      -3.151 105.196  17.101  1.00137.27           C
ATOM   1071  NH1 ARG D   3      -3.027 105.302  15.783  1.00136.09           N
ATOM   1072  NH2 ARG D   3      -4.065 105.926  17.729  1.00137.17           N
ATOM   1073  N   GLU D   4       3.236 102.515  20.322  1.00119.46           N
ATOM   1074  CA  GLU D   4       4.656 102.241  20.083  1.00117.02           C
ATOM   1075  C   GLU D   4       5.127 101.124  21.033  1.00113.77           C
ATOM   1076  O   GLU D   4       5.979 100.304  20.676  1.00112.68           O
ATOM   1077  CB  GLU D   4       5.479 103.524  20.283  1.00120.10           C
ATOM   1078  CG  GLU D   4       4.987 104.663  19.391  1.00125.95           C
ATOM   1079  CD  GLU D   4       6.071 105.680  19.009  1.00129.44           C
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ATOM   1080  OE1 GLU D   4       6.490 106.502  19.860  1.00131.18           O
ATOM   1081  OE2 GLU D   4       6.509 105.652  17.839  1.00131.54           O
ATOM   1082  N   LEU D   5       4.576 101.115  22.247  1.00107.77           N
ATOM   1083  CA  LEU D   5       4.866 100.080  23.238  1.00100.20           C
ATOM   1084  C   LEU D   5       4.172  98.789  22.748  1.00101.89           C
ATOM   1085  O   LEU D   5       4.540  97.680  23.140  1.00103.23           O
ATOM   1086  CB  LEU D   5       4.292 100.486  24.607  1.00 89.57           C
ATOM   1087  CG  LEU D   5       4.171  99.393  25.678  1.00 82.95           C
ATOM   1088  CD1 LEU D   5       5.536  99.024  26.172  1.00 79.39           C
ATOM   1089  CD2 LEU D   5       3.338  99.860  26.837  1.00 78.40           C
ATOM   1090  N   ASP D   6       3.160  98.945  21.894  1.00103.15           N
ATOM   1091  CA  ASP D   6       2.414  97.808  21.365  1.00104.18           C
ATOM   1092  C   ASP D   6       3.096  97.197  20.153  1.00103.81           C
ATOM   1093  O   ASP D   6       2.785  96.074  19.743  1.00102.97           O
ATOM   1094  CB  ASP D   6       0.971  98.212  21.039  1.00108.00           C
ATOM   1095  CG  ASP D   6       0.074  98.200  22.274  1.00112.58           C
ATOM   1096  OD1 ASP D   6       0.237  97.269  23.096  1.00115.34           O
ATOM   1097  OD2 ASP D   6      -0.785  99.100  22.417  1.00114.32           O
ATOM   1098  N   GLU D   7       4.014  97.959  19.569  1.00104.18           N
ATOM   1099  CA  GLU D   7       4.799  97.481  18.439  1.00104.53           C
ATOM   1100  C   GLU D   7       5.713  96.462  19.118  1.00103.48           C
ATOM   1101  O   GLU D   7       5.970  95.376  18.591  1.00102.50           O
ATOM   1102  CB  GLU D   7       5.617  98.638  17.849  1.00106.95           C
ATOM   1103  CG  GLU D   7       4.776  99.656  17.087  1.00110.40           C
ATOM   1104  CD  GLU D   7       4.581  99.279  15.628  1.00113.03           C
ATOM   1105  OE1 GLU D   7       5.459  99.643  14.813  1.00114.03           O
ATOM   1106  OE2 GLU D   7       3.568  98.614  15.299  1.00113.25           O
ATOM   1107  N   LEU D   8       6.176  96.835  20.311  1.00100.91           N
ATOM   1108  CA  LEU D   8       7.043  95.997  21.135  1.00 96.57           C
ATOM   1109  C   LEU D   8       6.300  94.770  21.645  1.00 98.57           C
ATOM   1110  O   LEU D   8       6.724  93.638  21.424  1.00100.66           O
ATOM   1111  CB  LEU D   8       7.542  96.766  22.354  1.00 89.15           C
ATOM   1112  CG  LEU D   8       8.429  97.975  22.144  1.00 82.99           C
ATOM   1113  CD1 LEU D   8       8.744  98.566  23.495  1.00 78.33           C
ATOM   1114  CD2 LEU D   8       9.689  97.577  21.412  1.00 78.68           C
ATOM   1115  N   MET D   9       5.207  94.995  22.364  1.00 98.60           N
ATOM   1116  CA  MET D   9       4.448  93.877  22.891  1.00101.80           C
ATOM   1117  C   MET D   9       4.186  92.858  21.787  1.00102.97           C
ATOM   1118  O   MET D   9       4.132  91.649  22.040  1.00102.93           O
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ATOM   1119  CB  MET D   9       3.136  94.375  23.500  1.00104.99           C
ATOM   1120  CG  MET D   9       3.338  95.015  24.860  1.00106.99           C
ATOM   1121  SD  MET D   9       4.406  93.995  25.914  1.00107.55           S
ATOM   1122  CE  MET D   9       3.273  92.744  26.447  1.00108.44           C
ATOM   1123  N   ALA D  10       4.048  93.355  20.560  1.00102.71           N
ATOM   1124  CA  ALA D  10       3.801  92.510  19.397  1.00102.15           C
ATOM   1125  C   ALA D  10       5.039  91.707  18.967  1.00101.89           C
ATOM   1126  O   ALA D  10       4.906  90.592  18.466  1.00102.04           O
ATOM   1127  CB  ALA D  10       3.299  93.361  18.234  1.00 99.65           C
ATOM   1128  N   SER D  11       6.234  92.268  19.161  1.00101.68           N
ATOM   1129  CA  SER D  11       7.494  91.604  18.790  1.00100.63           C
ATOM   1130  C   SER D  11       7.695  90.245  19.463  1.00104.57           C
ATOM   1131  O   SER D  11       8.455  89.405  18.966  1.00104.79           O
ATOM   1132  CB  SER D  11       8.697  92.485  19.141  1.00 96.62           C
ATOM   1133  OG  SER D  11       8.655  93.731  18.478  1.00 92.87           O
ATOM   1134  N   LEU D  12       7.033  90.037  20.598  1.00106.92           N
ATOM   1135  CA  LEU D  12       7.154  88.781  21.337  1.00109.11           C
ATOM   1136  C   LEU D  12       5.963  87.877  21.013  1.00112.49           C
ATOM   1137  O   LEU D  12       5.917  86.712  21.421  1.00111.74           O
ATOM   1138  CB  LEU D  12       7.196  89.075  22.837  1.00108.48           C
ATOM   1139  CG  LEU D  12       8.137  90.203  23.254  1.00104.98           C
ATOM   1140  CD1 LEU D  12       7.520  90.980  24.395  1.00100.51           C
ATOM   1141  CD2 LEU D  12       9.489  89.632  23.634  1.00104.05           C
ATOM   1142  N   SER D  13       5.009  88.448  20.276  1.00115.55           N
ATOM   1143  CA  SER D  13       3.781  87.783  19.839  1.00119.71           C
ATOM   1144  C   SER D  13       2.695  87.664  20.918  1.00122.54           C
ATOM   1145  O   SER D  13       2.075  88.710  21.225  1.00123.57           O
ATOM   1146  CB  SER D  13       4.112  86.401  19.257  1.00118.83           C
ATOM   1147  OG  SER D  13       4.951  86.509  18.113  1.00118.69           O
ATOM   1148  OXT SER D  13       2.482  86.542  21.435  1.00124.00           O
TER    1149      SER D  13
ATOM   1086  N   THR F   2      12.618  96.446  47.265  1.00167.72           N
ATOM   1087  CA  THR F   2      13.892  96.405  46.489  1.00168.68           C
ATOM   1088  C   THR F   2      14.921  95.534  47.201  1.00168.68           C
ATOM   1089  O   THR F   2      15.977  95.221  46.647  1.00168.77           O
ATOM   1090  CB  THR F   2      14.477  97.825  46.307  1.00169.03           C
ATOM   1091  CG2 THR F   2      15.821  97.770  45.586  1.00169.26           C
ATOM   1092  OG1 THR F   2      13.563  98.626  45.545  1.00170.92           O
ATOM   1093  N   ARG F   3      14.607  95.142  48.431  1.00168.25           N
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ATOM   1094  CA  ARG F   3      15.506  94.304  49.213  1.00167.59           C
ATOM   1095  C   ARG F   3      15.429  92.866  48.694  1.00168.72           C
ATOM   1096  O   ARG F   3      16.417  92.131  48.745  1.00169.37           O
ATOM   1097  CB  ARG F   3      15.122  94.374  50.695  1.00165.45           C
ATOM   1098  CG  ARG F   3      16.317  94.416  51.642  1.00163.06           C
ATOM   1099  CD  ARG F   3      15.889  94.705  53.078  1.00161.21           C
ATOM   1100  NE  ARG F   3      15.607  96.119  53.329  1.00159.22           N
ATOM   1101  CZ  ARG F   3      15.015  96.572  54.430  1.00158.39           C
ATOM   1102  NH1 ARG F   3      14.639  95.720  55.375  1.00157.72           N
ATOM   1103  NH2 ARG F   3      14.812  97.874  54.598  1.00157.85           N
ATOM   1104  N   GLU F   4      14.255  92.484  48.184  1.00169.29           N
ATOM   1105  CA  GLU F   4      14.025  91.146  47.628  1.00168.31           C
ATOM   1106  C   GLU F   4      14.487  91.112  46.170  1.00167.94           C
ATOM   1107  O   GLU F   4      14.764  90.045  45.609  1.00166.98           O
ATOM   1108  CB  GLU F   4      12.540  90.787  47.687  1.00167.80           C
ATOM   1109  CG  GLU F   4      11.896  90.899  49.060  1.00167.27           C
ATOM   1110  CD  GLU F   4      10.579  90.140  49.139  1.00168.28           C
ATOM   1111  OE1 GLU F   4       9.703  90.366  48.276  1.00167.92           O
ATOM   1112  OE2 GLU F   4      10.420  89.316  50.065  1.00168.81           O
ATOM   1113  N   LEU F   5      14.553  92.296  45.567  1.00167.58           N
ATOM   1114  CA  LEU F   5      15.002  92.453  44.189  1.00167.99           C
ATOM   1115  C   LEU F   5      16.537  92.441  44.166  1.00169.16           C
ATOM   1116  O   LEU F   5      17.157  92.024  43.182  1.00168.77           O
ATOM   1117  CB  LEU F   5      14.478  93.774  43.624  1.00166.25           C
ATOM   1118  CG  LEU F   5      14.988  94.231  42.257  1.00165.05           C
ATOM   1119  CD1 LEU F   5      14.468  93.324  41.150  1.00163.55           C
ATOM   1120  CD2 LEU F   5      14.538  95.656  42.032  1.00164.01           C
ATOM   1121  N   ASP F   6      17.140  92.897  45.263  1.00169.94           N
ATOM   1122  CA  ASP F   6      18.595  92.933  45.391  1.00169.64           C
ATOM   1123  C   ASP F   6      19.138  91.563  45.758  1.00169.28           C
ATOM   1124  O   ASP F   6      20.317  91.278  45.546  1.00168.18           O
ATOM   1125  CB  ASP F   6      19.023  93.965  46.434  1.00170.12           C
ATOM   1126  CG  ASP F   6      18.893  95.385  45.925  1.00172.08           C
ATOM   1127  OD1 ASP F   6      19.227  95.615  44.741  1.00172.61           O
ATOM   1128  OD2 ASP F   6      18.470  96.269  46.701  1.00173.49           O
ATOM   1129  N   GLU F   7      18.272  90.725  46.321  1.00169.63           N
ATOM   1130  CA  GLU F   7      18.642  89.358  46.664  1.00169.36           C
ATOM   1131  C   GLU F   7      18.916  88.778  45.282  1.00169.37           C
ATOM   1132  O   GLU F   7      19.858  88.009  45.071  1.00169.25           O
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ATOM   1133  CB  GLU F   7      17.453  88.619  47.297  1.00169.43           C
ATOM   1134  CG  GLU F   7      16.960  89.198  48.617  1.00168.79           C
ATOM   1135  CD  GLU F   7      17.596  88.538  49.825  1.00168.60           C
ATOM   1136  OE1 GLU F   7      17.092  87.480  50.260  1.00167.14           O
ATOM   1137  OE2 GLU F   7      18.606  89.071  50.333  1.00168.56           O
ATOM   1138  N   LEU F   8      18.069  89.199  44.345  1.00168.60           N
ATOM   1139  CA  LEU F   8      18.125  88.783  42.951  1.00167.55           C
ATOM   1140  C   LEU F   8      19.321  89.384  42.207  1.00168.46           C
ATOM   1141  O   LEU F   8      20.059  88.662  41.530  1.00168.63           O
ATOM   1142  CB  LEU F   8      16.817  89.177  42.252  1.00164.51           C
ATOM   1143  CG  LEU F   8      15.527  88.563  42.814  1.00161.82           C
ATOM   1144  CD1 LEU F   8      14.310  89.243  42.215  1.00160.14           C
ATOM   1145  CD2 LEU F   8      15.500  87.079  42.514  1.00161.14           C
ATOM   1146  N   MET F   9      19.517  90.696  42.341  1.00169.27           N
ATOM   1147  CA  MET F   9      20.623  91.381  41.671  1.00170.34           C
ATOM   1148  C   MET F   9      21.990  90.920  42.196  1.00170.50           C
ATOM   1149  O   MET F   9      23.015  91.080  41.523  1.00170.08           O
ATOM   1150  CB  MET F   9      20.474  92.903  41.821  1.00171.17           C
ATOM   1151  CG  MET F   9      19.210  93.489  41.164  1.00172.23           C
ATOM   1152  SD  MET F   9      18.947  93.057  39.408  1.00173.00           S
ATOM   1153  CE  MET F   9      20.201  94.088  38.567  1.00172.02           C
ATOM   1154  N   ALA F  10      21.988  90.333  43.391  1.00170.19           N
ATOM   1155  CA  ALA F  10      23.204  89.820  44.021  1.00169.09           C
ATOM   1156  C   ALA F  10      23.472  88.382  43.568  1.00168.90           C
ATOM   1157  O   ALA F  10      24.601  87.896  43.636  1.00167.06           O
ATOM   1158  CB  ALA F  10      23.064  89.874  45.540  1.00167.81           C
ATOM   1159  N   SER F  11      22.421  87.707  43.109  1.00169.78           N
ATOM   1160  CA  SER F  11      22.528  86.331  42.633  1.00169.93           C
ATOM   1161  C   SER F  11      23.397  86.282  41.387  1.00171.22           C
ATOM   1162  O   SER F  11      24.118  85.313  41.152  1.00170.34           O
ATOM   1163  CB  SER F  11      21.141  85.771  42.307  1.00168.77           C
ATOM   1164  OG  SER F  11      20.351  85.639  43.473  1.00167.98           O
ATOM   1165  N   LEU F  12      23.313  87.341  40.589  1.00173.79           N
ATOM   1166  CA  LEU F  12      24.082  87.455  39.358  1.00176.17           C
ATOM   1167  C   LEU F  12      25.519  87.870  39.666  1.00178.24           C
ATOM   1168  O   LEU F  12      26.379  87.870  38.784  1.00179.14           O
ATOM   1169  CB  LEU F  12      23.418  88.481  38.435  1.00175.22           C
ATOM   1170  CG  LEU F  12      21.974  88.127  38.071  1.00174.35           C
ATOM   1171  CD1 LEU F  12      21.284  89.305  37.400  1.00173.85           C
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ATOM   1172  CD2 LEU F  12      21.982  86.906  37.169  1.00173.97           C
ATOM   1173  N   SER F  13      25.764  88.221  40.927  1.00179.16           N
ATOM   1174  CA  SER F  13      27.089  88.635  41.384  1.00178.97           C
ATOM   1175  C   SER F  13      27.485  90.007  40.842  1.00178.68           C
ATOM   1176  O   SER F  13      26.605  90.897  40.774  1.00178.20           O
ATOM   1177  CB  SER F  13      28.139  87.596  40.975  1.00178.14           C
ATOM   1178  OG  SER F  13      27.780  86.303  41.428  1.00177.41           O
ATOM   1179  OXT SER F  13      28.678  90.172  40.506  1.00178.07           O
TER    1180      SER F  13
HETATM    1  O   HOH C   4       0.063 105.370  24.026  0.50 44.46           O
HETATM    2  O   HOH C   6       4.059  85.123  29.006  1.00 68.21           O
HETATM    3  O   HOH C  13       2.443 118.002  27.213  1.00 68.32           O
HETATM    4  O   HOH C  15      -9.253 105.330  47.946  1.00 65.07           O
HETATM    5  O   HOH C  17       5.281 111.016  36.277  1.00 75.53           O
HETATM    6  O   HOH C  33      -6.271  97.901  44.910  1.00 66.09           O
HETATM    7  O   HOH C  36     -12.626 115.981  38.240  1.00 66.58           O
HETATM    8  O   HOH C  48      13.676 103.936  30.402  1.00 66.06           O
HETATM    9  O   HOH C  50      -4.258  92.939  31.040  1.00 57.20           O
HETATM   10  O   HOH C  79       5.798  82.614  25.107  1.00 72.80           O
HETATM   11  O   HOH C 106      -7.939 111.090  44.635  1.00 54.84           O
HETATM 1150  O   HOH D  37       2.384 105.217  19.682  1.00 71.42           O
HETATM 1151  O   HOH D 111      10.178  87.969  17.399  1.00 73.03           O
HETATM 1181  O   HOH F 105      11.710  93.548  46.450  1.00 87.72           O
END
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2. The Augmented FAT/Paxillin Complex (§3.1.2 Structures):

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ATOM      1  N   ILE C 909      -7.120  90.264  27.594  1.00 84.95           N
ATOM      2  CA  ILE C 909      -6.328  91.240  26.773  1.00 86.58           C
ATOM      3  C   ILE C 909      -6.742  92.707  26.925  1.00 85.87           C
ATOM      4  O   ILE C 909      -7.924  93.047  26.881  1.00 86.73           O
ATOM      5  CB  ILE C 909      -6.375  90.883  25.252  1.00 85.93           C
ATOM      6  CG1 ILE C 909      -5.547  91.908  24.460  1.00 84.17           C
ATOM      7  CG2 ILE C 909      -7.829  90.811  24.763  1.00 79.59           C
ATOM      8  CD1 ILE C 909      -5.233  91.508  23.026  1.00 82.55           C
ATOM      9  N   SER C 910      -5.760  93.584  27.092  1.00 85.82           N
ATOM     10  CA  SER C 910      -6.064  95.004  27.245  1.00 88.03           C
ATOM     11  C   SER C 910      -6.002  95.773  25.931  1.00 87.92           C
ATOM     12  O   SER C 910      -5.363  95.336  24.962  1.00 90.37           O
ATOM     13  CB  SER C 910      -5.117  95.644  28.260  1.00 87.19           C
ATOM     14  OG  SER C 910      -3.892  94.924  28.339  1.00 88.96           O
ATOM     15  N   PRO C 911      -6.707  96.919  25.869  1.00 85.92           N
ATOM     16  CA  PRO C 911      -6.692  97.727  24.649  1.00 82.06           C
ATOM     17  C   PRO C 911      -5.458  98.621  24.779  1.00 76.36           C
ATOM     18  O   PRO C 911      -4.891  98.763  25.878  1.00 72.62           O
ATOM     19  CB  PRO C 911      -8.003  98.513  24.750  1.00 81.26           C
ATOM     20  CG  PRO C 911      -8.052  98.813  26.204  1.00 83.81           C
ATOM     21  CD  PRO C 911      -7.705  97.441  26.818  1.00 84.68           C
ATOM     22  N   PRO C 912      -5.029  99.238  23.668  1.00 69.40           N
ATOM     23  CA  PRO C 912      -3.851 100.103  23.695  1.00 63.70           C
ATOM     24  C   PRO C 912      -3.917 101.091  24.857  1.00 60.56           C
ATOM     25  O   PRO C 912      -4.996 101.538  25.235  1.00 61.26           O
ATOM     26  CB  PRO C 912      -3.923 100.804  22.338  1.00 65.28           C
ATOM     27  CG  PRO C 912      -4.655  99.848  21.490  1.00 64.22           C
ATOM     28  CD  PRO C 912      -5.745  99.375  22.395  1.00 65.66           C
ATOM     29  N   PRO C 913      -2.763 101.438  25.446  1.00 58.77           N
ATOM     30  CA  PRO C 913      -2.797 102.386  26.571  1.00 61.24           C
ATOM     31  C   PRO C 913      -3.755 103.530  26.256  1.00 63.36           C
ATOM     32  O   PRO C 913      -3.840 103.956  25.109  1.00 67.19           O
ATOM     33  CB  PRO C 913      -1.349 102.849  26.685  1.00 59.78           C
ATOM     34  CG  PRO C 913      -0.577 101.661  26.222  1.00 59.63           C
ATOM     35  CD  PRO C 913      -1.386 101.084  25.074  1.00 59.35           C
ATOM     36  N   THR C 914      -4.458 104.042  27.266  1.00 65.08           N
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ATOM     37  CA  THR C 914      -5.436 105.093  27.011  1.00 69.04           C
ATOM     38  C   THR C 914      -4.815 106.370  26.491  1.00 73.88           C
ATOM     39  O   THR C 914      -3.717 106.786  26.919  1.00 72.02           O
ATOM     40  CB  THR C 914      -6.315 105.419  28.250  1.00 69.24           C
ATOM     41  CG2 THR C 914      -5.485 106.060  29.340  1.00 69.56           C
ATOM     42  OG1 THR C 914      -7.361 106.329  27.874  1.00 67.64           O
ATOM     43  N   ALA C 915      -5.531 106.964  25.535  1.00 76.34           N
ATOM     44  CA  ALA C 915      -5.106 108.193  24.885  1.00 78.39           C
ATOM     45  C   ALA C 915      -5.407 109.387  25.786  1.00 81.78           C
ATOM     46  O   ALA C 915      -4.725 110.418  25.718  1.00 84.63           O
ATOM     47  CB  ALA C 915      -5.821 108.341  23.538  1.00 73.31           C
ATOM     48  N   ASN C 916      -6.399 109.226  26.660  1.00 82.80           N
ATOM     49  CA  ASN C 916      -6.816 110.305  27.546  1.00 82.11           C
ATOM     50  C   ASN C 916      -5.834 110.665  28.679  1.00 79.48           C
ATOM     51  O   ASN C 916      -6.252 111.247  29.670  1.00 75.73           O
ATOM     52  CB  ASN C 916      -8.204 109.979  28.131  1.00 88.81           C
ATOM     53  CG  ASN C 916      -9.073 109.113  27.184  1.00 94.91           C
ATOM     54  ND2 ASN C 916      -9.575 107.988  27.704  1.00 96.94           N
ATOM     55  OD1 ASN C 916      -9.289 109.455  26.012  1.00 99.35           O
ATOM     56  N   LEU C 917      -4.549 110.328  28.531  1.00 76.82           N
ATOM     57  CA  LEU C 917      -3.513 110.651  29.529  1.00 76.15           C
ATOM     58  C   LEU C 917      -2.212 111.089  28.847  1.00 76.67           C
ATOM     59  O   LEU C 917      -1.728 110.419  27.941  1.00 78.80           O
ATOM     60  CB  LEU C 917      -3.179 109.444  30.403  1.00 78.46           C
ATOM     61  CG  LEU C 917      -4.159 108.769  31.351  1.00 80.00           C
ATOM     62  CD1 LEU C 917      -3.506 107.526  31.939  1.00 78.87           C
ATOM     63  CD2 LEU C 917      -4.546 109.731  32.447  1.00 85.50           C
ATOM     64  N   ASP C 918      -1.611 112.173  29.311  1.00 78.12           N
ATOM     65  CA  ASP C 918      -0.394 112.668  28.673  1.00 82.31           C
ATOM     66  C   ASP C 918       0.858 111.919  29.108  1.00 81.67           C
ATOM     67  O   ASP C 918       1.210 111.929  30.285  1.00 84.04           O
ATOM     68  CB  ASP C 918      -0.238 114.174  28.947  1.00 88.22           C
ATOM     69  CG  ASP C 918       1.043 114.760  28.347  1.00 94.03           C
ATOM     70  OD1 ASP C 918       2.096 114.097  28.473  1.00 98.43           O
ATOM     71  OD2 ASP C 918       1.002 115.882  27.776  1.00 97.26
O1-
ATOM     72  N   ARG C 919       1.552 111.315  28.140  1.00 77.81           N
ATOM     73  CA  ARG C 919       2.757 110.518  28.399  1.00 71.26           C
ATOM     74  C   ARG C 919       4.063 111.292  28.346  1.00 73.28           C
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ATOM     75  O   ARG C 919       5.138 110.691  28.354  1.00 77.64           O
ATOM     76  CB  ARG C 919       2.842 109.384  27.386  1.00 60.42           C
ATOM     77  CG  ARG C 919       1.550 108.657  27.167  1.00 57.11           C
ATOM     78  CD  ARG C 919       1.107 107.962  28.421  1.00 54.34           C
ATOM     79  NE  ARG C 919      -0.182 107.321  28.226  1.00 57.02           N
ATOM     80  CZ  ARG C 919      -0.705 106.445  29.072  1.00 55.74           C
ATOM     81  NH1 ARG C 919      -0.039 106.116  30.173  1.00 54.16
N1+
ATOM     82  NH2 ARG C 919      -1.874 105.878  28.794  1.00 54.13           N
ATOM     83  N   SER C 920       3.984 112.613  28.284  1.00 74.38           N
ATOM     84  CA  SER C 920       5.195 113.421  28.187  1.00 76.74           C
ATOM     85  C   SER C 920       6.091 113.252  29.365  1.00 75.30           C
ATOM     86  O   SER C 920       7.317 113.241  29.232  1.00 72.65           O
ATOM     87  CB  SER C 920       4.871 114.909  28.089  1.00 79.67           C
ATOM     88  OG  SER C 920       4.047 115.190  26.977  1.00 89.57           O
ATOM     89  N   ASN C 921       5.466 113.149  30.529  1.00 77.59           N
ATOM     90  CA  ASN C 921       6.220 113.042  31.761  1.00 80.00           C
ATOM     91  C   ASN C 921       5.910 111.775  32.547  1.00 79.61           C
ATOM     92  O   ASN C 921       6.108 111.720  33.763  1.00 83.99           O
ATOM     93  CB  ASN C 921       5.972 114.304  32.602  1.00 78.49           C
ATOM     94  CG  ASN C 921       6.493 115.567  31.912  1.00 79.04           C
ATOM     95  ND2 ASN C 921       5.604 116.532  31.661  1.00 74.33           N
ATOM     96  OD1 ASN C 921       7.684 115.660  31.596  1.00 79.77           O
ATOM     97  N   ASP C 922       5.440 110.756  31.831  1.00 73.79           N
ATOM     98  CA  ASP C 922       5.106 109.470  32.427  1.00 70.09           C
ATOM     99  C   ASP C 922       6.337 108.555  32.462  1.00 69.92           C
ATOM    100  O   ASP C 922       6.608 107.825  31.504  1.00 71.98           O
ATOM    101  CB  ASP C 922       3.996 108.781  31.630  1.00 65.82           C
ATOM    102  CG  ASP C 922       3.281 107.715  32.440  1.00 66.60           C
ATOM    103  OD1 ASP C 922       3.871 107.216  33.425  1.00 64.17           O
ATOM    104  OD2 ASP C 922       2.130 107.378  32.093  1.00 68.31
O1-
ATOM    105  N   LYS C 923       7.085 108.609  33.559  1.00 67.80           N
ATOM    106  CA  LYS C 923       8.267 107.779  33.713  1.00 66.08           C
ATOM    107  C   LYS C 923       7.884 106.297  33.809  1.00 62.54           C
ATOM    108  O   LYS C 923       8.695 105.440  33.505  1.00 65.36           O
ATOM    109  CB  LYS C 923       9.080 108.228  34.942  1.00 67.57           C
ATOM    110  CG  LYS C 923      10.228 109.196  34.620  1.00 73.58           C
ATOM    111  CD  LYS C 923      11.553 108.468  34.336  1.00 78.66           C
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ATOM    112  CE  LYS C 923      12.152 107.810  35.606  1.00 85.47           C
ATOM    113  NZ  LYS C 923      13.465 107.085  35.397  1.00 79.94
N1+
ATOM    114  N   VAL C 924       6.661 105.978  34.222  1.00 57.97           N
ATOM    115  CA  VAL C 924       6.266 104.569  34.284  1.00 59.25           C
ATOM    116  C   VAL C 924       6.178 103.993  32.855  1.00 60.92           C
ATOM    117  O   VAL C 924       6.643 102.879  32.595  1.00 60.50           O
ATOM    118  CB  VAL C 924       4.903 104.386  35.012  1.00 59.50           C
ATOM    119  CG1 VAL C 924       4.414 102.937  34.899  1.00 51.04           C
ATOM    120  CG2 VAL C 924       5.065 104.748  36.465  1.00 55.92           C
ATOM    121  N   TYR C 925       5.578 104.768  31.947  1.00 59.17           N
ATOM    122  CA  TYR C 925       5.413 104.412  30.538  1.00 58.27           C
ATOM    123  C   TYR C 925       6.798 104.265  29.891  1.00 62.45           C
ATOM    124  O   TYR C 925       7.025 103.397  29.044  1.00 61.60           O
ATOM    125  CB  TYR C 925       4.613 105.514  29.839  1.00 54.96           C
ATOM    126  CG  TYR C 925       3.947 105.102  28.554  1.00 54.96           C
ATOM    127  CD1 TYR C 925       4.609 105.202  27.336  1.00 58.50           C
ATOM    128  CD2 TYR C 925       2.659 104.582  28.559  1.00 58.34           C
ATOM    129  CE1 TYR C 925       4.003 104.793  26.144  1.00 59.20           C
ATOM    130  CE2 TYR C 925       2.039 104.161  27.376  1.00 58.79           C
ATOM    131  CZ  TYR C 925       2.721 104.270  26.171  1.00 60.73           C
ATOM    132  OH  TYR C 925       2.130 103.849  25.001  1.00 57.74           O
ATOM    133  N   GLU C 926       7.725 105.123  30.299  1.00 65.25           N
ATOM    134  CA  GLU C 926       9.083 105.089  29.780  1.00 68.80           C
ATOM    135  C   GLU C 926       9.809 103.861  30.320  1.00 69.97           C
ATOM    136  O   GLU C 926      10.430 103.099  29.570  1.00 69.90           O
ATOM    137  CB  GLU C 926       9.820 106.358  30.202  1.00 75.59           C
ATOM    138  CG  GLU C 926      11.293 106.408  29.819  1.00 90.96           C
ATOM    139  CD  GLU C 926      11.965 107.723  30.223  1.00101.09           C
ATOM    140  OE1 GLU C 926      11.383 108.464  31.050  1.00109.17           O
ATOM    141  OE2 GLU C 926      13.079 108.010  29.724  1.00106.84
O1-
ATOM    142  N   ASN C 927       9.717 103.666  31.629  1.00 68.66           N
ATOM    143  CA  ASN C 927      10.376 102.541  32.254  1.00 67.67           C
ATOM    144  C   ASN C 927       9.822 101.200  31.828  1.00 68.74           C
ATOM    145  O   ASN C 927      10.574 100.227  31.768  1.00 72.39           O
ATOM    146  CB  ASN C 927      10.352 102.684  33.773  1.00 68.05           C
ATOM    147  CG  ASN C 927      11.327 103.738  34.259  1.00 70.92           C
ATOM    148  ND2 ASN C 927      11.334 103.976  35.562  1.00 70.63           N
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ATOM    149  OD1 ASN C 927      12.072 104.335  33.465  1.00 69.96           O
ATOM    150  N   VAL C 928       8.523 101.126  31.546  1.00 64.92           N
ATOM    151  CA  VAL C 928       7.941  99.868  31.076  1.00 61.66           C
ATOM    152  C   VAL C 928       8.547  99.631  29.700  1.00 60.07           C
ATOM    153  O   VAL C 928       9.082  98.562  29.420  1.00 60.30           O
ATOM    154  CB  VAL C 928       6.392  99.942  30.981  1.00 60.82           C
ATOM    155  CG1 VAL C 928       5.872  98.889  30.022  1.00 60.29           C
ATOM    156  CG2 VAL C 928       5.771  99.725  32.365  1.00 58.20           C
ATOM    157  N   THR C 929       8.485 100.652  28.851  1.00 63.07           N
ATOM    158  CA  THR C 929       9.054 100.578  27.512  1.00 61.40           C
ATOM    159  C   THR C 929      10.504 100.131  27.584  1.00 62.87           C
ATOM    160  O   THR C 929      10.971  99.358  26.749  1.00 63.14           O
ATOM    161  CB  THR C 929       9.003 101.927  26.841  1.00 58.88           C
ATOM    162  CG2 THR C 929       9.757 101.909  25.557  1.00 63.85           C
ATOM    163  OG1 THR C 929       7.646 102.254  26.554  1.00 62.34           O
ATOM    164  N   GLY C 930      11.216 100.623  28.589  1.00 64.51           N
ATOM    165  CA  GLY C 930      12.602 100.244  28.739  1.00 64.78           C
ATOM    166  C   GLY C 930      12.737  98.768  29.037  1.00 68.72           C
ATOM    167  O   GLY C 930      13.534  98.079  28.411  1.00 73.17           O
ATOM    168  N   LEU C 931      11.958  98.289  30.002  1.00 71.25           N
ATOM    169  CA  LEU C 931      11.973  96.891  30.393  1.00 69.93           C
ATOM    170  C   LEU C 931      11.542  96.037  29.233  1.00 66.95           C
ATOM    171  O   LEU C 931      12.208  95.065  28.914  1.00 67.13           O
ATOM    172  CB  LEU C 931      11.026  96.633  31.565  1.00 73.68           C
ATOM    173  CG  LEU C 931      10.990  95.208  32.125  1.00 77.88           C
ATOM    174  CD1 LEU C 931      12.404  94.755  32.513  1.00 77.15           C
ATOM    175  CD2 LEU C 931      10.054  95.182  33.332  1.00 79.64           C
ATOM    176  N   VAL C 932      10.424  96.365  28.603  1.00 65.09           N
ATOM    177  CA  VAL C 932      10.009  95.537  27.488  1.00 69.46           C
ATOM    178  C   VAL C 932      11.164  95.398  26.517  1.00 73.87           C
ATOM    179  O   VAL C 932      11.497  94.297  26.098  1.00 72.32           O
ATOM    180  CB  VAL C 932       8.820  96.110  26.756  1.00 63.05           C
ATOM    181  CG1 VAL C 932       8.589  95.329  25.483  1.00 62.98           C
ATOM    182  CG2 VAL C 932       7.609  96.025  27.642  1.00 59.58           C
ATOM    183  N   LYS C 933      11.776  96.530  26.185  1.00 79.21           N
ATOM    184  CA  LYS C 933      12.912  96.599  25.274  1.00 80.58           C
ATOM    185  C   LYS C 933      14.141  95.773  25.707  1.00 83.29           C
ATOM    186  O   LYS C 933      14.731  95.054  24.891  1.00 83.49           O
ATOM    187  CB  LYS C 933      13.294  98.064  25.107  1.00 81.60           C
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ATOM    188  CG  LYS C 933      13.286  98.550  23.670  1.00 84.45           C
ATOM    189  CD  LYS C 933      12.877 100.009  23.543  1.00 84.61           C
ATOM    190  CE  LYS C 933      11.568 100.112  22.774  1.00 83.57           C
ATOM    191  NZ  LYS C 933      11.236 101.508  22.371  1.00 88.80
N1+
ATOM    192  N   ALA C 934      14.542  95.872  26.973  1.00 83.91           N
ATOM    193  CA  ALA C 934      15.700  95.101  27.431  1.00 86.68           C
ATOM    194  C   ALA C 934      15.429  93.604  27.294  1.00 88.36           C
ATOM    195  O   ALA C 934      16.351  92.809  27.107  1.00 92.75           O
ATOM    196  CB  ALA C 934      16.048  95.439  28.880  1.00 87.14           C
ATOM    197  N   VAL C 935      14.159  93.227  27.407  1.00 85.45           N
ATOM    198  CA  VAL C 935      13.733  91.839  27.268  1.00 81.49           C
ATOM    199  C   VAL C 935      13.888  91.417  25.814  1.00 81.92           C
ATOM    200  O   VAL C 935      14.375  90.328  25.520  1.00 83.58           O
ATOM    201  CB  VAL C 935      12.247  91.673  27.699  1.00 79.53           C
ATOM    202  CG1 VAL C 935      11.545  90.605  26.852  1.00 72.69           C
ATOM    203  CG2 VAL C 935      12.184  91.310  29.164  1.00 75.15           C
ATOM    204  N   ILE C 936      13.469  92.291  24.910  1.00 82.93           N
ATOM    205  CA  ILE C 936      13.551  92.020  23.489  1.00 85.97           C
ATOM    206  C   ILE C 936      15.010  91.975  23.021  1.00 92.14           C
ATOM    207  O   ILE C 936      15.336  91.325  22.022  1.00 90.57           O
ATOM    208  CB  ILE C 936      12.766  93.078  22.709  1.00 80.76           C
ATOM    209  CG1 ILE C 936      11.295  93.014  23.104  1.00 78.23           C
ATOM    210  CG2 ILE C 936      12.879  92.827  21.232  1.00 82.49           C
ATOM    211  CD1 ILE C 936      10.444  94.028  22.396  1.00 76.28           C
ATOM    212  N   GLU C 937      15.891  92.658  23.746  1.00 98.38           N
ATOM    213  CA  GLU C 937      17.309  92.662  23.401  1.00105.29           C
ATOM    214  C   GLU C 937      17.875  91.261  23.702  1.00106.70           C
ATOM    215  O   GLU C 937      18.752  90.751  22.996  1.00109.35           O
ATOM    216  CB  GLU C 937      18.034  93.754  24.208  1.00109.34           C
ATOM    217  CG  GLU C 937      19.500  93.990  23.811  1.00114.00           C
ATOM    218  CD  GLU C 937      19.745  93.851  22.306  1.00117.38           C
ATOM    219  OE1 GLU C 937      18.904  94.339  21.512  1.00115.32           O
ATOM    220  OE2 GLU C 937      20.785  93.257  21.925  1.00117.56
O1-
ATOM    221  N   MET C 938      17.361  90.644  24.761  1.00108.24           N
ATOM    222  CA  MET C 938      17.762  89.296  25.136  1.00107.56           C
ATOM    223  C   MET C 938      16.978  88.301  24.275  1.00108.86           C
ATOM    224  O   MET C 938      17.521  87.303  23.809  1.00107.20           O
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ATOM    225  CB  MET C 938      17.444  89.039  26.605  1.00103.15           C
ATOM    226  CG  MET C 938      17.085  87.600  26.890  1.00100.99           C
ATOM    227  SD  MET C 938      16.864  87.280  28.638  1.00102.23           S
ATOM    228  CE  MET C 938      18.424  87.925  29.302  1.00 96.91           C
ATOM    229  N   SER C 939      15.696  88.584  24.061  1.00112.38           N
ATOM    230  CA  SER C 939      14.840  87.692  23.279  1.00117.67           C
ATOM    231  C   SER C 939      15.323  87.446  21.848  1.00119.77           C
ATOM    232  O   SER C 939      15.197  86.328  21.338  1.00118.72           O
ATOM    233  CB  SER C 939      13.392  88.216  23.235  1.00118.43           C
ATOM    234  OG  SER C 939      13.138  88.966  22.054  1.00120.19           O
ATOM    235  N   SER C 940      15.871  88.474  21.200  1.00122.53           N
ATOM    236  CA  SER C 940      16.335  88.328  19.820  1.00124.52           C
ATOM    237  C   SER C 940      17.828  88.067  19.662  1.00125.63           C
ATOM    238  O   SER C 940      18.302  87.764  18.559  1.00123.74           O
ATOM    239  CB  SER C 940      15.955  89.558  19.002  1.00124.34           C
ATOM    240  OG  SER C 940      16.234  89.323  17.633  1.00124.58           O
ATOM    241  N   LYS C 941      18.561  88.199  20.763  1.00127.31           N
ATOM    242  CA  LYS C 941      19.995  87.954  20.756  1.00130.31           C
ATOM    243  C   LYS C 941      20.260  86.516  21.259  1.00133.31           C
ATOM    244  O   LYS C 941      20.191  85.556  20.483  1.00134.26           O
ATOM    245  CB  LYS C 941      20.706  88.985  21.646  1.00129.68           C
ATOM    246  CG  LYS C 941      22.179  89.203  21.304  1.00133.13           C
ATOM    247  CD  LYS C 941      23.024  87.947  21.534  1.00136.10           C
ATOM    248  CE  LYS C 941      24.242  87.899  20.601  1.00136.33           C
ATOM    249  NZ  LYS C 941      25.034  89.168  20.595  1.00133.87
N1+
ATOM    250  N   ILE C 942      20.531  86.399  22.563  1.00135.72           N
ATOM    251  CA  ILE C 942      20.832  85.149  23.304  1.00135.88           C
ATOM    252  C   ILE C 942      20.989  83.747  22.671  1.00135.69           C
ATOM    253  O   ILE C 942      21.954  83.048  23.011  1.00136.41           O
ATOM    254  CB  ILE C 942      19.861  84.953  24.508  1.00135.80           C
ATOM    255  CG1 ILE C 942      20.569  84.151  25.618  1.00134.32           C
ATOM    256  CG2 ILE C 942      18.583  84.210  24.062  1.00133.16           C
ATOM    257  CD1 ILE C 942      19.708  83.865  26.818  1.00133.90           C
ATOM    258  N   GLN C 943      20.075  83.315  21.798  1.00134.34           N
ATOM    259  CA  GLN C 943      20.188  81.993  21.193  1.00132.88           C
ATOM    260  C   GLN C 943      21.674  81.652  21.016  1.00132.35           C
ATOM    261  O   GLN C 943      22.173  80.690  21.625  1.00132.00           O
ATOM    262  CB  GLN C 943      19.414  81.962  19.851  1.00132.04           C
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ATOM    263  CG  GLN C 943      17.982  81.446  20.006  1.00131.86           C
ATOM    264  CD  GLN C 943      17.936  79.947  20.263  1.00131.58           C
ATOM    265  NE2 GLN C 943      17.400  79.551  21.420  1.00128.52           N
ATOM    266  OE1 GLN C 943      18.384  79.155  19.431  1.00131.63           O
ATOM    267  N   PRO C 944      22.408  82.449  20.194  1.00131.19           N
ATOM    268  CA  PRO C 944      23.835  82.210  19.966  1.00127.40           C
ATOM    269  C   PRO C 944      24.699  82.162  21.238  1.00124.05           C
ATOM    270  O   PRO C 944      25.070  81.116  21.760  1.00122.03           O
ATOM    271  CB  PRO C 944      24.201  83.391  19.093  1.00128.29           C
ATOM    272  CG  PRO C 944      23.087  83.384  18.151  1.00129.04           C
ATOM    273  CD  PRO C 944      21.968  83.466  19.213  1.00130.52           C
ATOM    274  N   ALA C 945      24.992  83.349  21.743  1.00122.53           N
ATOM    275  CA  ALA C 945      25.806  83.568  22.946  1.00122.04           C
ATOM    276  C   ALA C 945      25.841  82.540  24.075  1.00120.54           C
ATOM    277  O   ALA C 945      24.840  81.906  24.400  1.00119.65           O
ATOM    278  CB  ALA C 945      25.494  84.961  23.538  1.00121.84           C
ATOM    279  N   PRO C 946      27.033  82.368  24.685  1.00120.48           N
ATOM    280  CA  PRO C 946      27.308  81.442  25.797  1.00120.10           C
ATOM    281  C   PRO C 946      27.088  82.176  27.137  1.00118.51           C
ATOM    282  O   PRO C 946      26.599  83.308  27.138  1.00117.33           O
ATOM    283  CB  PRO C 946      28.772  81.055  25.571  1.00121.49           C
ATOM    284  CG  PRO C 946      29.366  82.309  24.986  1.00120.89           C
ATOM    285  CD  PRO C 946      28.288  82.759  24.011  1.00120.40           C
ATOM    286  N   PRO C 947      27.429  81.554  28.284  1.00118.59           N
ATOM    287  CA  PRO C 947      27.252  82.190  29.601  1.00120.40           C
ATOM    288  C   PRO C 947      28.096  83.451  29.875  1.00122.86           C
ATOM    289  O   PRO C 947      27.870  84.150  30.863  1.00121.93           O
ATOM    290  CB  PRO C 947      27.594  81.069  30.570  1.00119.50           C
ATOM    291  CG  PRO C 947      27.130  79.871  29.861  1.00118.56           C
ATOM    292  CD  PRO C 947      27.576  80.097  28.434  1.00118.85           C
ATOM    293  N   GLU C 948      29.105  83.725  29.052  1.00126.09           N
ATOM    294  CA  GLU C 948      29.921  84.935  29.256  1.00128.05           C
ATOM    295  C   GLU C 948      29.179  86.102  28.618  1.00129.22           C
ATOM    296  O   GLU C 948      29.651  87.246  28.633  1.00129.11           O
ATOM    297  CB  GLU C 948      31.281  84.804  28.563  1.00128.79           C
ATOM    298  CG  GLU C 948      32.407  84.236  29.412  1.00129.22           C
ATOM    299  CD  GLU C 948      33.351  83.374  28.595  1.00129.49           C
ATOM    300  OE1 GLU C 948      34.515  83.783  28.369  1.00127.95           O
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ATOM    301  OE2 GLU C 948      32.907  82.282  28.171  1.00130.34
O1-
ATOM    302  N   GLU C 949      27.998  85.811  28.081  1.00130.67           N
ATOM    303  CA  GLU C 949      27.249  86.828  27.372  1.00132.06           C
ATOM    304  C   GLU C 949      25.753  87.036  27.699  1.00131.00           C
ATOM    305  O   GLU C 949      25.239  88.139  27.493  1.00130.08           O
ATOM    306  CB  GLU C 949      27.510  86.591  25.880  1.00134.83           C
ATOM    307  CG  GLU C 949      29.022  86.702  25.559  1.00139.33           C
ATOM    308  CD  GLU C 949      29.411  86.198  24.172  1.00142.36           C
ATOM    309  OE1 GLU C 949      28.784  86.638  23.181  1.00144.45           O
ATOM    310  OE2 GLU C 949      30.356  85.376  24.080  1.00140.95
O1-
ATOM    311  N   TYR C 950      25.041  86.011  28.181  1.00129.73           N
ATOM    312  CA  TYR C 950      23.648  86.241  28.575  1.00125.37           C
ATOM    313  C   TYR C 950      23.553  86.517  30.088  1.00123.89           C
ATOM    314  O   TYR C 950      22.607  87.168  30.529  1.00124.67           O
ATOM    315  CB  TYR C 950      22.678  85.099  28.172  1.00124.27           C
ATOM    316  CG  TYR C 950      23.065  83.664  28.475  1.00124.30           C
ATOM    317  CD1 TYR C 950      23.439  83.256  29.757  1.00123.25           C
ATOM    318  CD2 TYR C 950      22.993  82.694  27.471  1.00123.52           C
ATOM    319  CE1 TYR C 950      23.729  81.904  30.027  1.00122.44           C
ATOM    320  CE2 TYR C 950      23.276  81.354  27.728  1.00122.74           C
ATOM    321  CZ  TYR C 950      23.645  80.961  29.000  1.00123.33           C
ATOM    322  OH  TYR C 950      23.933  79.628  29.219  1.00122.73           O
ATOM    323  N   VAL C 951      24.527  86.057  30.879  1.00121.89           N
ATOM    324  CA  VAL C 951      24.483  86.321  32.314  1.00122.76           C
ATOM    325  C   VAL C 951      24.330  87.824  32.567  1.00126.35           C
ATOM    326  O   VAL C 951      23.721  88.226  33.566  1.00128.44           O
ATOM    327  CB  VAL C 951      25.731  85.811  33.041  1.00121.55           C
ATOM    328  CG1 VAL C 951      25.719  86.295  34.493  1.00119.27           C
ATOM    329  CG2 VAL C 951      25.732  84.296  33.010  1.00122.16           C
ATOM    330  N   PRO C 952      24.913  88.677  31.687  1.00127.99           N
ATOM    331  CA  PRO C 952      24.782  90.131  31.868  1.00126.63           C
ATOM    332  C   PRO C 952      23.495  90.571  31.136  1.00125.51           C
ATOM    333  O   PRO C 952      22.759  91.421  31.623  1.00124.87           O
ATOM    334  CB  PRO C 952      26.048  90.694  31.202  1.00126.03           C
ATOM    335  CG  PRO C 952      27.016  89.550  31.238  1.00127.51           C
ATOM    336  CD  PRO C 952      26.122  88.382  30.895  1.00128.76           C
ATOM    337  N   MET C 953      23.236  89.989  29.960  1.00124.90           N
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ATOM    338  CA  MET C 953      22.025  90.287  29.161  1.00124.90           C
ATOM    339  C   MET C 953      20.768  90.152  30.033  1.00123.24           C
ATOM    340  O   MET C 953      19.695  90.642  29.674  1.00123.57           O
ATOM    341  CB  MET C 953      21.900  89.307  27.982  1.00128.34           C
ATOM    342  CG  MET C 953      21.893  89.921  26.586  1.00132.89           C
ATOM    343  SD  MET C 953      21.585  88.654  25.299  1.00139.20           S
ATOM    344  CE  MET C 953      23.116  87.639  25.355  1.00133.99           C
ATOM    345  N   VAL C 954      20.914  89.433  31.149  1.00120.10           N
ATOM    346  CA  VAL C 954      19.851  89.218  32.134  1.00115.86           C
ATOM    347  C   VAL C 954      20.044  90.326  33.162  1.00114.76           C
ATOM    348  O   VAL C 954      19.100  91.026  33.523  1.00115.64           O
ATOM    349  CB  VAL C 954      19.980  87.827  32.841  1.00115.37           C
ATOM    350  CG1 VAL C 954      19.528  87.912  34.295  1.00114.62           C
ATOM    351  CG2 VAL C 954      19.132  86.800  32.120  1.00111.15           C
ATOM    352  N   LYS C 955      21.281  90.484  33.625  1.00112.03           N
ATOM    353  CA  LYS C 955      21.611  91.524  34.594  1.00110.08           C
ATOM    354  C   LYS C 955      20.988  92.853  34.129  1.00108.57           C
ATOM    355  O   LYS C 955      20.634  93.707  34.946  1.00107.99           O
ATOM    356  CB  LYS C 955      23.136  91.641  34.715  1.00109.26           C
ATOM    357  CG  LYS C 955      23.618  92.778  35.592  1.00112.85           C
ATOM    358  CD  LYS C 955      23.180  92.635  37.038  1.00113.69           C
ATOM    359  CE  LYS C 955      23.684  93.818  37.851  1.00117.31           C
ATOM    360  NZ  LYS C 955      23.412  93.674  39.305  1.00120.85
N1+
ATOM    361  N   GLU C 956      20.849  93.000  32.810  1.00106.12           N
ATOM    362  CA  GLU C 956      20.259  94.183  32.181  1.00104.23           C
ATOM    363  C   GLU C 956      18.766  94.254  32.481  1.00101.34           C
ATOM    364  O   GLU C 956      18.304  95.191  33.132  1.00101.80           O
ATOM    365  CB  GLU C 956      20.462  94.139  30.661  1.00107.40           C
ATOM    366  CG  GLU C 956      21.683  94.881  30.150  1.00115.30           C
ATOM    367  CD  GLU C 956      21.296  96.029  29.238  1.00120.67           C
ATOM    368  OE1 GLU C 956      20.256  95.899  28.554  1.00123.99           O
ATOM    369  OE2 GLU C 956      22.023  97.048  29.192  1.00123.79
O1-
ATOM    370  N   VAL C 957      18.018  93.275  31.974  1.00 97.84           N
ATOM    371  CA  VAL C 957      16.575  93.179  32.202  1.00 91.30           C
ATOM    372  C   VAL C 957      16.287  93.287  33.705  1.00 89.63           C
ATOM    373  O   VAL C 957      15.201  93.722  34.111  1.00 89.13           O
ATOM    374  CB  VAL C 957      16.024  91.823  31.670  1.00 86.99           C
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ATOM    375  CG1 VAL C 957      14.696  91.487  32.325  1.00 81.87           C
ATOM    376  CG2 VAL C 957      15.859  91.885  30.162  1.00 83.49           C
ATOM    377  N   GLY C 958      17.258  92.877  34.521  1.00 86.73           N
ATOM    378  CA  GLY C 958      17.100  92.942  35.963  1.00 86.30           C
ATOM    379  C   GLY C 958      17.253  94.357  36.489  1.00 87.09           C
ATOM    380  O   GLY C 958      16.602  94.736  37.470  1.00 87.61           O
ATOM    381  N   LEU C 959      18.122  95.134  35.836  1.00 88.08           N
ATOM    382  CA  LEU C 959      18.390  96.533  36.203  1.00 87.22           C
ATOM    383  C   LEU C 959      17.248  97.427  35.696  1.00 84.42           C
ATOM    384  O   LEU C 959      16.860  98.399  36.361  1.00 81.73           O
ATOM    385  CB  LEU C 959      19.752  96.998  35.617  1.00 90.23           C
ATOM    386  CG  LEU C 959      21.069  96.402  36.183  1.00 94.61           C
ATOM    387  CD1 LEU C 959      22.235  96.526  35.174  1.00 91.08           C
ATOM    388  CD2 LEU C 959      21.416  97.110  37.493  1.00 96.47           C
ATOM    389  N   ALA C 960      16.710  97.079  34.525  1.00 80.88           N
ATOM    390  CA  ALA C 960      15.614  97.822  33.912  1.00 78.40           C
ATOM    391  C   ALA C 960      14.308  97.632  34.678  1.00 77.74           C
ATOM    392  O   ALA C 960      13.397  98.449  34.574  1.00 77.60           O
ATOM    393  CB  ALA C 960      15.435  97.385  32.474  1.00 77.27           C
ATOM    394  N   LEU C 961      14.216  96.536  35.424  1.00 77.06           N
ATOM    395  CA  LEU C 961      13.037  96.242  36.225  1.00 75.44           C
ATOM    396  C   LEU C 961      13.202  96.911  37.577  1.00 77.45           C
ATOM    397  O   LEU C 961      12.229  97.333  38.204  1.00 76.85           O
ATOM    398  CB  LEU C 961      12.883  94.737  36.432  1.00 73.48           C
ATOM    399  CG  LEU C 961      11.791  94.360  37.440  1.00 72.22           C
ATOM    400  CD1 LEU C 961      10.410  94.596  36.828  1.00 67.24           C
ATOM    401  CD2 LEU C 961      11.961  92.903  37.858  1.00 73.06           C
ATOM    402  N   ARG C 962      14.440  96.984  38.042  1.00 81.45           N
ATOM    403  CA  ARG C 962      14.714  97.632  39.314  1.00 86.24           C
ATOM    404  C   ARG C 962      14.209  99.069  39.193  1.00 83.35           C
ATOM    405  O   ARG C 962      13.524  99.572  40.085  1.00 83.50           O
ATOM    406  CB  ARG C 962      16.218  97.617  39.594  1.00 96.72           C
ATOM    407  CG  ARG C 962      16.627  98.192  40.952  1.00107.84           C
ATOM    408  CD  ARG C 962      18.157  98.202  41.147  1.00114.40           C
ATOM    409  NE  ARG C 962      18.488  98.556  42.529  1.00123.62           N
ATOM    410  CZ  ARG C 962      19.715  98.810  42.983  1.00127.32           C
ATOM    411  NH1 ARG C 962      20.761  98.751  42.164  1.00129.36
N1+
ATOM    412  NH2 ARG C 962      19.890  99.139  44.262  1.00127.50           N
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ATOM    413  N   THR C 963      14.550  99.700  38.066  1.00 81.04           N
ATOM    414  CA  THR C 963      14.159 101.075  37.737  1.00 77.34           C
ATOM    415  C   THR C 963      12.641 101.222  37.673  1.00 76.41           C
ATOM    416  O   THR C 963      12.077 102.135  38.271  1.00 78.85           O
ATOM    417  CB  THR C 963      14.703 101.532  36.342  1.00 77.75           C
ATOM    418  CG2 THR C 963      14.212 102.939  36.011  1.00 73.04           C
ATOM    419  OG1 THR C 963      16.136 101.527  36.336  1.00 76.39           O
ATOM    420  N   LEU C 964      11.984 100.333  36.931  1.00 72.53           N
ATOM    421  CA  LEU C 964      10.537 100.405  36.784  1.00 71.29           C
ATOM    422  C   LEU C 964       9.855 100.296  38.114  1.00 71.98           C
ATOM    423  O   LEU C 964       8.906 101.030  38.397  1.00 72.44           O
ATOM    424  CB  LEU C 964      10.006  99.298  35.868  1.00 68.42           C
ATOM    425  CG  LEU C 964       8.478  99.135  35.810  1.00 64.26           C
ATOM    426  CD1 LEU C 964       7.791 100.441  35.463  1.00 57.94           C
ATOM    427  CD2 LEU C 964       8.152  98.068  34.782  1.00 62.07           C
ATOM    428  N   LEU C 965      10.341  99.370  38.931  1.00 74.48           N
ATOM    429  CA  LEU C 965       9.764  99.152  40.246  1.00 75.89           C
ATOM    430  C   LEU C 965       9.991 100.384  41.094  1.00 74.88           C
ATOM    431  O   LEU C 965       9.085 100.824  41.815  1.00 73.74           O
ATOM    432  CB  LEU C 965      10.368  97.896  40.879  1.00 76.31           C
ATOM    433  CG  LEU C 965       9.876  96.665  40.106  1.00 76.66           C
ATOM    434  CD1 LEU C 965      10.606  95.443  40.588  1.00 76.56           C
ATOM    435  CD2 LEU C 965       8.357  96.507  40.275  1.00 75.94           C
ATOM    436  N   ALA C 966      11.190 100.954  40.972  1.00 72.90           N
ATOM    437  CA  ALA C 966      11.550 102.167  41.701  1.00 71.93           C
ATOM    438  C   ALA C 966      10.582 103.315  41.362  1.00 70.46           C
ATOM    439  O   ALA C 966      10.082 103.991  42.268  1.00 72.48           O
ATOM    440  CB  ALA C 966      12.976 102.562  41.371  1.00 69.12           C
ATOM    441  N   THR C 967      10.313 103.520  40.070  1.00 67.44           N
ATOM    442  CA  THR C 967       9.398 104.565  39.627  1.00 63.01           C
ATOM    443  C   THR C 967       7.976 104.304  40.072  1.00 64.40           C
ATOM    444  O   THR C 967       7.271 105.235  40.454  1.00 65.31           O
ATOM    445  CB  THR C 967       9.358 104.693  38.112  1.00 64.08           C
ATOM    446  CG2 THR C 967       8.359 105.741  37.688  1.00 64.42           C
ATOM    447  OG1 THR C 967      10.644 105.078  37.638  1.00 67.54           O
ATOM    448  N   VAL C 968       7.524 103.056  40.012  1.00 63.53           N
ATOM    449  CA  VAL C 968       6.156 102.809  40.440  1.00 65.67           C
ATOM    450  C   VAL C 968       6.079 103.144  41.926  1.00 69.31           C
ATOM    451  O   VAL C 968       5.044 103.603  42.400  1.00 68.50           O
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ATOM    452  CB  VAL C 968       5.682 101.338  40.194  1.00 64.11           C
ATOM    453  CG1 VAL C 968       4.207 101.203  40.574  1.00 57.49           C
ATOM    454  CG2 VAL C 968       5.860 100.949  38.731  1.00 60.33           C
ATOM    455  N   ASP C 969       7.181 102.944  42.650  1.00 75.56           N
ATOM    456  CA  ASP C 969       7.206 103.246  44.080  1.00 83.87           C
ATOM    457  C   ASP C 969       7.015 104.739  44.334  1.00 87.31           C
ATOM    458  O   ASP C 969       6.393 105.127  45.328  1.00 90.96           O
ATOM    459  CB  ASP C 969       8.512 102.774  44.730  1.00 90.65           C
ATOM    460  CG  ASP C 969       8.646 101.247  44.743  1.00 99.31           C
ATOM    461  OD1 ASP C 969       7.585 100.569  44.687  1.00 99.15           O
ATOM    462  OD2 ASP C 969       9.804 100.741  44.822  1.00102.67
O1-
ATOM    463  N   GLU C 970       7.551 105.579  43.451  1.00 87.78           N
ATOM    464  CA  GLU C 970       7.383 107.025  43.592  1.00 87.87           C
ATOM    465  C   GLU C 970       6.020 107.494  43.066  1.00 86.64           C
ATOM    466  O   GLU C 970       5.565 108.587  43.390  1.00 89.18           O
ATOM    467  CB  GLU C 970       8.467 107.757  42.828  1.00 87.52           C
ATOM    468  CG  GLU C 970       9.852 107.398  43.245  1.00 98.17           C
ATOM    469  CD  GLU C 970      10.886 108.142  42.426  1.00107.97           C
ATOM    470  OE1 GLU C 970      10.958 107.886  41.196  1.00110.90           O
ATOM    471  OE2 GLU C 970      11.615 108.980  43.015  1.00110.97
O1-
ATOM    472  N   THR C 971       5.355 106.657  42.284  1.00 82.40           N
ATOM    473  CA  THR C 971       4.087 107.046  41.711  1.00 79.25           C
ATOM    474  C   THR C 971       2.865 106.634  42.512  1.00 80.67           C
ATOM    475  O   THR C 971       1.841 107.311  42.466  1.00 81.99           O
ATOM    476  CB  THR C 971       3.993 106.485  40.276  1.00 79.59           C
ATOM    477  CG2 THR C 971       2.685 106.873  39.595  1.00 75.08           C
ATOM    478  OG1 THR C 971       5.091 106.996  39.512  1.00 72.72           O
ATOM    479  N   ILE C 972       2.962 105.531  43.244  1.00 81.67           N
ATOM    480  CA  ILE C 972       1.817 105.045  44.024  1.00 83.42           C
ATOM    481  C   ILE C 972       1.269 106.051  45.048  1.00 80.81           C
ATOM    482  O   ILE C 972       0.046 106.236  45.160  1.00 74.87           O
ATOM    483  CB  ILE C 972       2.166 103.743  44.776  1.00 83.46           C
ATOM    484  CG1 ILE C 972       2.802 102.745  43.820  1.00 84.93           C
ATOM    485  CG2 ILE C 972       0.902 103.090  45.323  1.00 83.58           C
ATOM    486  CD1 ILE C 972       3.825 101.854  44.487  1.00 89.93           C
ATOM    487  N   PRO C 973       2.169 106.709  45.805  1.00 79.99           N
ATOM    488  CA  PRO C 973       1.744 107.687  46.814  1.00 79.69           C
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ATOM    489  C   PRO C 973       0.568 108.529  46.339  1.00 80.30           C
ATOM    490  O   PRO C 973      -0.466 108.639  47.004  1.00 81.02           O
ATOM    491  CB  PRO C 973       2.995 108.535  47.016  1.00 76.57           C
ATOM    492  CG  PRO C 973       4.097 107.565  46.802  1.00 75.19           C
ATOM    493  CD  PRO C 973       3.637 106.739  45.625  1.00 76.30           C
ATOM    494  N   LEU C 974       0.765 109.106  45.162  1.00 77.51           N
ATOM    495  CA  LEU C 974      -0.186 109.972  44.493  1.00 75.93           C
ATOM    496  C   LEU C 974      -1.568 109.412  44.101  1.00 74.44           C
ATOM    497  O   LEU C 974      -2.544 110.144  44.073  1.00 75.32           O
ATOM    498  CB  LEU C 974       0.491 110.533  43.243  1.00 76.44           C
ATOM    499  CG  LEU C 974      -0.441 111.137  42.189  1.00 80.68           C
ATOM    500  CD1 LEU C 974      -0.996 112.470  42.673  1.00 80.27           C
ATOM    501  CD2 LEU C 974       0.336 111.310  40.882  1.00 84.93           C
ATOM    502  N   LEU C 975      -1.675 108.129  43.801  1.00 73.62           N
ATOM    503  CA  LEU C 975      -2.967 107.620  43.354  1.00 75.01           C
ATOM    504  C   LEU C 975      -3.926 107.317  44.492  1.00 74.03           C
ATOM    505  O   LEU C 975      -3.518 107.273  45.653  1.00 75.19           O
ATOM    506  CB  LEU C 975      -2.734 106.391  42.475  1.00 75.34           C
ATOM    507  CG  LEU C 975      -1.607 106.735  41.489  1.00 78.17           C
ATOM    508  CD1 LEU C 975      -0.730 105.515  41.226  1.00 79.70           C
ATOM    509  CD2 LEU C 975      -2.208 107.321  40.208  1.00 79.20           C
ATOM    510  N   PRO C 976      -5.222 107.135  44.178  1.00 72.08           N
ATOM    511  CA  PRO C 976      -6.211 106.835  45.216  1.00 74.16           C
ATOM    512  C   PRO C 976      -5.691 105.762  46.154  1.00 75.80           C
ATOM    513  O   PRO C 976      -4.933 104.894  45.741  1.00 79.03           O
ATOM    514  CB  PRO C 976      -7.413 106.388  44.405  1.00 72.85           C
ATOM    515  CG  PRO C 976      -7.355 107.346  43.252  1.00 69.07           C
ATOM    516  CD  PRO C 976      -5.882 107.359  42.880  1.00 68.30           C
ATOM    517  N   ALA C 977      -6.082 105.823  47.421  1.00 80.66           N
ATOM    518  CA  ALA C 977      -5.611 104.827  48.381  1.00 80.60           C
ATOM    519  C   ALA C 977      -6.081 103.447  47.977  1.00 79.40           C
ATOM    520  O   ALA C 977      -5.274 102.504  47.939  1.00 78.47           O
ATOM    521  CB  ALA C 977      -6.120 105.152  49.803  1.00 79.02           C
ATOM    522  N   SER C 978      -7.378 103.357  47.658  1.00 77.53           N
ATOM    523  CA  SER C 978      -8.031 102.094  47.311  1.00 79.82           C
ATOM    524  C   SER C 978      -7.295 101.299  46.265  1.00 83.07           C
ATOM    525  O   SER C 978      -7.200 100.076  46.359  1.00 88.50           O
ATOM    526  CB  SER C 978      -9.484 102.323  46.851  1.00 77.34           C
ATOM    527  OG  SER C 978      -9.563 102.906  45.566  1.00 79.95           O
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ATOM    528  N   THR C 979      -6.742 101.997  45.285  1.00 82.72           N
ATOM    529  CA  THR C 979      -6.036 101.333  44.206  1.00 77.91           C
ATOM    530  C   THR C 979      -4.576 100.906  44.454  1.00 78.02           C
ATOM    531  O   THR C 979      -3.975 100.280  43.582  1.00 79.71           O
ATOM    532  CB  THR C 979      -6.049 102.220  42.970  1.00 74.94           C
ATOM    533  CG2 THR C 979      -7.463 102.693  42.648  1.00 62.47           C
ATOM    534  OG1 THR C 979      -5.230 103.361  43.230  1.00 75.64           O
ATOM    535  N   HIS C 980      -3.995 101.207  45.610  1.00 77.48           N
ATOM    536  CA  HIS C 980      -2.596 100.836  45.805  1.00 79.32           C
ATOM    537  C   HIS C 980      -2.347  99.360  45.884  1.00 78.62           C
ATOM    538  O   HIS C 980      -1.223  98.914  45.667  1.00 76.26           O
ATOM    539  CB  HIS C 980      -2.002 101.472  47.063  1.00 82.98           C
ATOM    540  CG  HIS C 980      -1.892 102.959  46.997  1.00 84.15           C
ATOM    541  CD2 HIS C 980      -2.532 103.867  46.227  1.00 85.49           C
ATOM    542  ND1 HIS C 980      -1.043 103.678  47.815  1.00 85.84           N
ATOM    543  CE1 HIS C 980      -1.170 104.960  47.550  1.00 89.89           C
ATOM    544  NE2 HIS C 980      -2.067 105.111  46.591  1.00 88.60           N
ATOM    545  N   ARG C 981      -3.393  98.604  46.194  1.00 80.21           N
ATOM    546  CA  ARG C 981      -3.273  97.156  46.350  1.00 83.54           C
ATOM    547  C   ARG C 981      -3.079  96.385  45.028  1.00 81.92           C
ATOM    548  O   ARG C 981      -2.167  95.556  44.928  1.00 82.24           O
ATOM    549  CB  ARG C 981      -4.497  96.638  47.135  1.00 85.47           C
ATOM    550  CG  ARG C 981      -4.421  95.184  47.647  1.00 84.60           C
ATOM    551  CD  ARG C 981      -3.350  94.950  48.715  1.00 81.06           C
ATOM    552  NE  ARG C 981      -3.156  93.514  48.938  1.00 83.61           N
ATOM    553  CZ  ARG C 981      -2.444  92.979  49.927  1.00 82.35           C
ATOM    554  NH1 ARG C 981      -1.841  93.759  50.811  1.00 80.71
N1+
ATOM    555  NH2 ARG C 981      -2.345  91.657  50.034  1.00 79.63           N
ATOM    556  N   GLU C 982      -3.914  96.656  44.022  1.00 80.43           N
ATOM    557  CA  GLU C 982      -3.786  95.974  42.731  1.00 79.47           C
ATOM    558  C   GLU C 982      -2.404  96.311  42.154  1.00 76.02           C
ATOM    559  O   GLU C 982      -1.742  95.468  41.549  1.00 71.51           O
ATOM    560  CB  GLU C 982      -4.898  96.413  41.748  1.00 80.96           C
ATOM    561  CG  GLU C 982      -5.503  95.242  40.900  1.00 92.71           C
ATOM    562  CD  GLU C 982      -6.581  95.659  39.837  1.00100.52           C
ATOM    563  OE1 GLU C 982      -7.568  96.362  40.206  1.00102.24           O
ATOM    564  OE2 GLU C 982      -6.445  95.262  38.642  1.00 95.96
O1-
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ATOM    565  N   ILE C 983      -1.949  97.532  42.392  1.00 70.78           N
ATOM    566  CA  ILE C 983      -0.664  97.950  41.858  1.00 72.18           C
ATOM    567  C   ILE C 983       0.518  97.342  42.579  1.00 74.15           C
ATOM    568  O   ILE C 983       1.570  97.112  41.982  1.00 77.23           O
ATOM    569  CB  ILE C 983      -0.499  99.493  41.882  1.00 70.97           C
ATOM    570  CG1 ILE C 983      -1.659 100.156  41.129  1.00 66.21           C
ATOM    571  CG2 ILE C 983       0.847  99.874  41.255  1.00 64.06           C
ATOM    572  CD1 ILE C 983      -1.696 101.652  41.230  1.00 60.12           C
ATOM    573  N   GLU C 984       0.365  97.091  43.868  1.00 77.02           N
ATOM    574  CA  GLU C 984       1.468  96.517  44.618  1.00 79.38           C
ATOM    575  C   GLU C 984       1.536  95.055  44.225  1.00 77.09           C
ATOM    576  O   GLU C 984       2.611  94.471  44.090  1.00 74.08           O
ATOM    577  CB  GLU C 984       1.222  96.681  46.119  1.00 88.11           C
ATOM    578  CG  GLU C 984       2.184  97.655  46.801  1.00 99.14           C
ATOM    579  CD  GLU C 984       1.475  98.580  47.793  1.00109.11           C
ATOM    580  OE1 GLU C 984       0.546  98.103  48.497  1.00115.25           O
ATOM    581  OE2 GLU C 984       1.856  99.777  47.871  1.00110.47
O1-
ATOM    582  N   MET C 985       0.361  94.481  44.016  1.00 73.92           N
ATOM    583  CA  MET C 985       0.245  93.099  43.614  1.00 70.59           C
ATOM    584  C   MET C 985       0.861  92.887  42.213  1.00 69.46           C
ATOM    585  O   MET C 985       1.607  91.926  42.001  1.00 66.72           O
ATOM    586  CB  MET C 985      -1.233  92.703  43.675  1.00 72.71           C
ATOM    587  CG  MET C 985      -1.492  91.613  44.708  1.00 80.42           C
ATOM    588  SD  MET C 985      -0.766  91.853  46.390  1.00 85.30           S
ATOM    589  CE  MET C 985       1.105  91.464  46.198  1.00 82.08           C
ATOM    590  N   ALA C 986       0.546  93.791  41.273  1.00 69.08           N
ATOM    591  CA  ALA C 986       1.086  93.766  39.907  1.00 61.06           C
ATOM    592  C   ALA C 986       2.615  93.820  39.977  1.00 61.60           C
ATOM    593  O   ALA C 986       3.303  93.201  39.182  1.00 60.41           O
ATOM    594  CB  ALA C 986       0.572  94.944  39.135  1.00 52.88           C
ATOM    595  N   GLN C 987       3.150  94.579  40.923  1.00 64.40           N
ATOM    596  CA  GLN C 987       4.599  94.650  41.083  1.00 69.94           C
ATOM    597  C   GLN C 987       5.205  93.350  41.620  1.00 74.21           C
ATOM    598  O   GLN C 987       6.300  92.942  41.218  1.00 74.81           O
ATOM    599  CB  GLN C 987       4.983  95.727  42.075  1.00 73.29           C
ATOM    600  CG  GLN C 987       4.787  97.131  41.646  1.00 74.46           C
ATOM    601  CD  GLN C 987       5.230  98.082  42.734  1.00 74.15           C
ATOM    602  NE2 GLN C 987       6.511  98.466  42.700  1.00 69.51           N
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ATOM    603  OE1 GLN C 987       4.443  98.447  43.616  1.00 71.07           O
ATOM    604  N   LYS C 988       4.530  92.725  42.579  1.00 75.72           N
ATOM    605  CA  LYS C 988       5.067  91.498  43.139  1.00 76.85           C
ATOM    606  C   LYS C 988       5.101  90.456  42.035  1.00 74.61           C
ATOM    607  O   LYS C 988       6.022  89.629  41.960  1.00 75.89           O
ATOM    608  CB  LYS C 988       4.220  91.014  44.326  1.00 83.11           C
ATOM    609  CG  LYS C 988       4.609  89.609  44.824  1.00 93.91           C
ATOM    610  CD  LYS C 988       6.140  89.444  45.039  1.00 98.59           C
ATOM    611  CE  LYS C 988       6.550  87.970  45.192  1.00 96.94           C
ATOM    612  NZ  LYS C 988       7.178  87.683  46.513  1.00101.06
N1+
ATOM    613  N   LEU C 989       4.100  90.506  41.167  1.00 67.38           N
ATOM    614  CA  LEU C 989       4.039  89.571  40.066  1.00 63.95           C
ATOM    615  C   LEU C 989       5.287  89.710  39.200  1.00 63.62           C
ATOM    616  O   LEU C 989       5.862  88.713  38.787  1.00 63.80           O
ATOM    617  CB  LEU C 989       2.782  89.822  39.246  1.00 60.47           C
ATOM    618  CG  LEU C 989       2.464  88.855  38.113  1.00 57.38           C
ATOM    619  CD1 LEU C 989       2.515  87.434  38.615  1.00 56.34           C
ATOM    620  CD2 LEU C 989       1.091  89.182  37.565  1.00 54.02           C
ATOM    621  N   LEU C 990       5.711  90.940  38.928  1.00 63.58           N
ATOM    622  CA  LEU C 990       6.906  91.159  38.119  1.00 63.56           C
ATOM    623  C   LEU C 990       8.165  90.600  38.784  1.00 64.92           C
ATOM    624  O   LEU C 990       9.055  90.093  38.096  1.00 62.19           O
ATOM    625  CB  LEU C 990       7.084  92.645  37.830  1.00 61.74           C
ATOM    626  CG  LEU C 990       6.074  93.214  36.848  1.00 60.69           C
ATOM    627  CD1 LEU C 990       6.124  94.706  36.887  1.00 60.66           C
ATOM    628  CD2 LEU C 990       6.384  92.706  35.467  1.00 63.00           C
ATOM    629  N   ASN C 991       8.238  90.707  40.111  1.00 67.78           N
ATOM    630  CA  ASN C 991       9.373  90.189  40.880  1.00 73.14           C
ATOM    631  C   ASN C 991       9.567  88.705  40.638  1.00 73.68           C
ATOM    632  O   ASN C 991      10.670  88.249  40.299  1.00 74.98           O
ATOM    633  CB  ASN C 991       9.158  90.403  42.380  1.00 78.47           C
ATOM    634  CG  ASN C 991       9.744  91.706  42.865  1.00 84.33           C
ATOM    635  ND2 ASN C 991       8.906  92.539  43.479  1.00 87.31           N
ATOM    636  OD1 ASN C 991      10.947  91.965  42.695  1.00 84.79           O
ATOM    637  N   SER C 992       8.486  87.952  40.832  1.00 74.02           N
ATOM    638  CA  SER C 992       8.518  86.516  40.634  1.00 72.44           C
ATOM    639  C   SER C 992       8.788  86.152  39.168  1.00 70.80           C
ATOM    640  O   SER C 992       9.392  85.115  38.911  1.00 71.78           O
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ATOM    641  CB  SER C 992       7.216  85.887  41.120  1.00 68.96           C
ATOM    642  OG  SER C 992       6.140  86.325  40.325  1.00 75.27           O
ATOM    643  N   ASP C 993       8.359  86.984  38.213  1.00 71.52           N
ATOM    644  CA  ASP C 993       8.626  86.706  36.793  1.00 72.93           C
ATOM    645  C   ASP C 993      10.134  86.756  36.544  1.00 75.63           C
ATOM    646  O   ASP C 993      10.654  86.008  35.705  1.00 78.90           O
ATOM    647  CB  ASP C 993       7.941  87.725  35.871  1.00 71.56           C
ATOM    648  CG  ASP C 993       6.431  87.555  35.824  1.00 77.47           C
ATOM    649  OD1 ASP C 993       5.900  86.632  36.481  1.00 82.03           O
ATOM    650  OD2 ASP C 993       5.768  88.348  35.125  1.00 81.94
O1-
ATOM    651  N   LEU C 994      10.823  87.653  37.259  1.00 74.25           N
ATOM    652  CA  LEU C 994      12.268  87.804  37.142  1.00 73.89           C
ATOM    653  C   LEU C 994      12.936  86.630  37.832  1.00 77.39           C
ATOM    654  O   LEU C 994      14.002  86.163  37.408  1.00 77.56           O
ATOM    655  CB  LEU C 994      12.743  89.084  37.805  1.00 73.64           C
ATOM    656  CG  LEU C 994      14.220  89.291  37.510  1.00 71.58           C
ATOM    657  CD1 LEU C 994      14.368  89.691  36.055  1.00 71.16           C
ATOM    658  CD2 LEU C 994      14.777  90.357  38.418  1.00 74.31           C
ATOM    659  N   GLY C 995      12.322  86.184  38.924  1.00 77.11           N
ATOM    660  CA  GLY C 995      12.842  85.034  39.630  1.00 76.87           C
ATOM    661  C   GLY C 995      12.807  83.852  38.671  1.00 76.99           C
ATOM    662  O   GLY C 995      13.779  83.106  38.601  1.00 79.72           O
ATOM    663  N   GLU C 996      11.710  83.681  37.926  1.00 74.12           N
ATOM    664  CA  GLU C 996      11.604  82.574  36.970  1.00 75.44           C
ATOM    665  C   GLU C 996      12.772  82.677  35.997  1.00 75.09           C
ATOM    666  O   GLU C 996      13.544  81.740  35.846  1.00 73.31           O
ATOM    667  CB  GLU C 996      10.274  82.632  36.199  1.00 73.95           C
ATOM    668  CG  GLU C 996       9.818  81.301  35.556  1.00 73.82           C
ATOM    669  CD  GLU C 996       8.433  81.395  34.888  1.00 77.98           C
ATOM    670  OE1 GLU C 996       7.448  81.779  35.563  1.00 75.02           O
ATOM    671  OE2 GLU C 996       8.325  81.077  33.680  1.00 77.06
O1-
ATOM    672  N   LEU C 997      12.903  83.835  35.358  1.00 78.06           N
ATOM    673  CA  LEU C 997      13.975  84.087  34.404  1.00 78.32           C
ATOM    674  C   LEU C 997      15.374  83.765  34.937  1.00 78.80           C
ATOM    675  O   LEU C 997      16.201  83.205  34.217  1.00 77.85           O
ATOM    676  CB  LEU C 997      13.936  85.542  33.958  1.00 77.28           C
ATOM    677  CG  LEU C 997      15.135  85.949  33.111  1.00 76.64           C
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ATOM    678  CD1 LEU C 997      15.128  85.187  31.794  1.00 73.66           C
ATOM    679  CD2 LEU C 997      15.080  87.437  32.882  1.00 75.03           C
ATOM    680  N   ILE C 998      15.641  84.120  36.189  1.00 77.25           N
ATOM    681  CA  ILE C 998      16.947  83.856  36.778  1.00 80.31           C
ATOM    682  C   ILE C 998      17.186  82.371  37.048  1.00 83.04           C
ATOM    683  O   ILE C 998      18.311  81.881  36.886  1.00 84.10           O
ATOM    684  CB  ILE C 998      17.140  84.687  38.064  1.00 79.40           C
ATOM    685  CG1 ILE C 998      17.338  86.155  37.670  1.00 82.60           C
ATOM    686  CG2 ILE C 998      18.340  84.181  38.859  1.00 77.20           C
ATOM    687  CD1 ILE C 998      16.937  87.149  38.742  1.00 82.48           C
ATOM    688  N   ASN C 999      16.130  81.663  37.448  1.00 83.79           N
ATOM    689  CA  ASN C 999      16.215  80.231  37.715  1.00 80.31           C
ATOM    690  C   ASN C 999      16.506  79.513  36.407  1.00 80.21           C
ATOM    691  O   ASN C 999      17.221  78.514  36.394  1.00 79.90           O
ATOM    692  CB  ASN C 999      14.897  79.681  38.276  1.00 81.63           C
ATOM    693  CG  ASN C 999      14.604  80.160  39.685  1.00 83.96           C
ATOM    694  ND2 ASN C 999      13.329  80.125  40.071  1.00 82.73           N
ATOM    695  OD1 ASN C 999      15.513  80.536  40.426  1.00 87.64           O
ATOM    696  N   LYS C1000      15.939  80.012  35.310  1.00 79.78           N
ATOM    697  CA  LYS C1000      16.156  79.384  34.018  1.00 82.69           C
ATOM    698  C   LYS C1000      17.539  79.701  33.523  1.00 87.29           C
ATOM    699  O   LYS C1000      18.087  78.965  32.713  1.00 91.27           O
ATOM    700  CB  LYS C1000      15.121  79.835  32.986  1.00 81.29           C
ATOM    701  CG  LYS C1000      13.688  79.470  33.362  1.00 83.64           C
ATOM    702  CD  LYS C1000      13.614  78.121  34.082  1.00 82.20           C
ATOM    703  CE  LYS C1000      12.198  77.667  34.392  1.00 78.59           C
ATOM    704  NZ  LYS C1000      12.266  76.569  35.393  1.00 79.19
N1+
ATOM    705  N   MET C1001      18.111  80.801  34.001  1.00 90.75           N
ATOM    706  CA  MET C1001      19.462  81.159  33.594  1.00 90.87           C
ATOM    707  C   MET C1001      20.436  80.267  34.379  1.00 90.41           C
ATOM    708  O   MET C1001      21.204  79.502  33.786  1.00 86.93           O
ATOM    709  CB  MET C1001      19.746  82.633  33.887  1.00 91.75           C
ATOM    710  CG  MET C1001      21.171  83.040  33.555  1.00 96.80           C
ATOM    711  SD  MET C1001      21.772  84.462  34.507  1.00104.71           S
ATOM    712  CE  MET C1001      22.116  83.736  36.195  1.00102.20           C
ATOM    713  N   LYS C1002      20.397  80.370  35.709  1.00 87.99           N
ATOM    714  CA  LYS C1002      21.254  79.563  36.573  1.00 89.70           C
ATOM    715  C   LYS C1002      21.318  78.115  36.066  1.00 92.93           C
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ATOM    716  O   LYS C1002      22.354  77.457  36.171  1.00 96.73           O
ATOM    717  CB  LYS C1002      20.728  79.572  38.015  1.00 87.91           C
ATOM    718  CG  LYS C1002      21.259  80.674  38.936  1.00 88.01           C
ATOM    719  CD  LYS C1002      20.895  80.339  40.397  1.00 93.03           C
ATOM    720  CE  LYS C1002      21.721  81.109  41.441  1.00 97.29           C
ATOM    721  NZ  LYS C1002      21.562  82.593  41.386  1.00 99.06
N1+
ATOM    722  N   LEU C1003      20.206  77.622  35.522  1.00 95.37           N
ATOM    723  CA  LEU C1003      20.147  76.259  34.994  1.00 96.66           C
ATOM    724  C   LEU C1003      20.899  76.139  33.678  1.00 98.82           C
ATOM    725  O   LEU C1003      21.751  75.275  33.542  1.00101.68           O
ATOM    726  CB  LEU C1003      18.698  75.791  34.775  1.00 95.97           C
ATOM    727  CG  LEU C1003      17.827  75.312  35.947  1.00 93.54           C
ATOM    728  CD1 LEU C1003      16.393  75.124  35.463  1.00 86.75           C
ATOM    729  CD2 LEU C1003      18.380  74.017  36.524  1.00 89.52           C
ATOM    730  N   ALA C1004      20.595  76.992  32.705  1.00100.95           N
ATOM    731  CA  ALA C1004      21.287  76.907  31.416  1.00103.86           C
ATOM    732  C   ALA C1004      22.817  77.076  31.577  1.00105.77           C
ATOM    733  O   ALA C1004      23.599  76.756  30.667  1.00106.40           O
ATOM    734  CB  ALA C1004      20.717  77.949  30.448  1.00 99.99           C
ATOM    735  N   GLN C1005      23.230  77.565  32.746  1.00104.01           N
ATOM    736  CA  GLN C1005      24.641  77.766  33.051  1.00101.96           C
ATOM    737  C   GLN C1005      25.242  76.479  33.553  1.00101.55           C
ATOM    738  O   GLN C1005      26.385  76.148  33.251  1.00103.75           O
ATOM    739  CB  GLN C1005      24.813  78.829  34.124  1.00101.05           C
ATOM    740  CG  GLN C1005      24.698  80.210  33.593  1.00104.56           C
ATOM    741  CD  GLN C1005      25.625  81.136  34.306  1.00106.03           C
ATOM    742  NE2 GLN C1005      26.756  81.434  33.674  1.00106.95           N
ATOM    743  OE1 GLN C1005      25.346  81.575  35.425  1.00107.39           O
ATOM    744  N   GLN C1006      24.458  75.772  34.349  1.00 98.97           N
ATOM    745  CA  GLN C1006      24.866  74.510  34.917  1.00 96.86           C
ATOM    746  C   GLN C1006      24.851  73.431  33.834  1.00 96.20           C
ATOM    747  O   GLN C1006      25.409  72.350  34.030  1.00 96.22           O
ATOM    748  CB  GLN C1006      23.912  74.172  36.063  1.00 97.68           C
ATOM    749  CG  GLN C1006      24.048  72.801  36.671  1.00102.93           C
ATOM    750  CD  GLN C1006      23.163  72.647  37.901  1.00107.56           C
ATOM    751  NE2 GLN C1006      23.495  71.685  38.754  1.00109.99           N
ATOM    752  OE1 GLN C1006      22.186  73.382  38.076  1.00110.02           O
ATOM    753  N   TYR C1007      24.228  73.730  32.693  1.00 96.63           N
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ATOM    754  CA  TYR C1007      24.142  72.762  31.599  1.00101.98           C
ATOM    755  C   TYR C1007      24.628  73.311  30.265  1.00106.08           C
ATOM    756  O   TYR C1007      23.866  73.388  29.297  1.00105.01           O
ATOM    757  CB  TYR C1007      22.700  72.226  31.454  1.00102.62           C
ATOM    758  CG  TYR C1007      22.205  71.480  32.678  1.00100.68           C
ATOM    759  CD1 TYR C1007      21.822  72.170  33.824  1.00100.14           C
ATOM    760  CD2 TYR C1007      22.223  70.087  32.729  1.00 99.33           C
ATOM    761  CE1 TYR C1007      21.485  71.504  34.990  1.00 98.40           C
ATOM    762  CE2 TYR C1007      21.887  69.408  33.900  1.00 99.82           C
ATOM    763  CZ  TYR C1007      21.521  70.127  35.027  1.00 99.31           C
ATOM    764  OH  TYR C1007      21.209  69.483  36.204  1.00 97.57           O
ATOM    765  N   VAL C1008      25.908  73.689  30.226  1.00112.40           N
ATOM    766  CA  VAL C1008      26.529  74.230  29.009  1.00115.62           C
ATOM    767  C   VAL C1008      27.091  73.120  28.101  1.00118.68           C
ATOM    768  O   VAL C1008      27.695  72.137  28.578  1.00117.20           O
ATOM    769  CB  VAL C1008      27.686  75.220  29.327  1.00113.43           C
ATOM    770  CG1 VAL C1008      27.885  76.188  28.144  1.00111.71           C
ATOM    771  CG2 VAL C1008      27.398  75.965  30.605  1.00110.31           C
ATOM    772  N   MET C1009      26.904  73.311  26.792  1.00119.55           N
ATOM    773  CA  MET C1009      27.340  72.355  25.773  1.00120.49           C
ATOM    774  C   MET C1009      26.614  71.033  26.043  1.00119.74           C
ATOM    775  O   MET C1009      27.248  69.978  26.202  1.00119.45           O
ATOM    776  CB  MET C1009      28.865  72.122  25.825  1.00122.89           C
ATOM    777  CG  MET C1009      29.740  73.355  25.576  1.00121.78           C
ATOM    778  SD  MET C1009      31.003  73.589  26.868  1.00126.30           S
ATOM    779  CE  MET C1009      31.538  71.843  27.253  1.00121.09           C
ATOM    780  N   THR C1010      25.283  71.103  26.109  1.00117.79           N
ATOM    781  CA  THR C1010      24.447  69.925  26.363  1.00112.34           C
ATOM    782  C   THR C1010      23.162  70.041  25.546  1.00109.06           C
ATOM    783  O   THR C1010      22.902  71.063  24.904  1.00107.42           O
ATOM    784  CB  THR C1010      24.040  69.810  27.873  1.00110.10           C
ATOM    785  CG2 THR C1010      23.531  68.420  28.191  1.00110.33           C
ATOM    786  OG1 THR C1010      25.175  70.047  28.712  1.00105.49           O
ATOM    787  N   SER C1011      22.369  68.980  25.563  1.00106.23           N
ATOM    788  CA  SER C1011      21.088  68.985  24.876  1.00106.87           C
ATOM    789  C   SER C1011      20.139  69.820  25.756  1.00107.19           C
ATOM    790  O   SER C1011      19.082  70.297  25.308  1.00102.61           O
ATOM    791  CB  SER C1011      20.578  67.549  24.762  1.00107.83           C
ATOM    792  OG  SER C1011      20.787  66.826  25.974  1.00104.56           O
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ATOM    793  N   LEU C1012      20.543  69.982  27.020  1.00107.60           N
ATOM    794  CA  LEU C1012      19.753  70.719  28.003  1.00107.90           C
ATOM    795  C   LEU C1012      19.973  72.207  27.945  1.00109.30           C
ATOM    796  O   LEU C1012      19.075  72.984  28.287  1.00110.31           O
ATOM    797  CB  LEU C1012      20.015  70.220  29.438  1.00104.23           C
ATOM    798  CG  LEU C1012      19.319  68.895  29.812  1.00103.41           C
ATOM    799  CD1 LEU C1012      19.096  68.867  31.327  1.00 99.74           C
ATOM    800  CD2 LEU C1012      17.969  68.739  29.062  1.00 97.65           C
ATOM    801  N   GLN C1013      21.164  72.600  27.505  1.00110.00           N
ATOM    802  CA  GLN C1013      21.506  74.009  27.394  1.00108.04           C
ATOM    803  C   GLN C1013      20.532  74.741  26.469  1.00104.48           C
ATOM    804  O   GLN C1013      20.138  75.874  26.739  1.00103.94           O
ATOM    805  CB  GLN C1013      22.928  74.158  26.862  1.00110.51           C
ATOM    806  CG  GLN C1013      23.373  75.603  26.716  1.00113.77           C
ATOM    807  CD  GLN C1013      24.452  75.747  25.670  1.00113.99           C
ATOM    808  NE2 GLN C1013      24.084  76.308  24.522  1.00112.15           N
ATOM    809  OE1 GLN C1013      25.600  75.339  25.876  1.00113.81           O
ATOM    810  N   GLN C1014      20.157  74.098  25.371  1.00102.14           N
ATOM    811  CA  GLN C1014      19.235  74.718  24.440  1.00100.91           C
ATOM    812  C   GLN C1014      17.838  74.778  25.043  1.00102.05           C
ATOM    813  O   GLN C1014      17.068  75.682  24.723  1.00104.42           O
ATOM    814  CB  GLN C1014      19.194  73.944  23.119  1.00102.30           C
ATOM    815  CG  GLN C1014      18.388  74.634  22.009  1.00110.82           C
ATOM    816  CD  GLN C1014      16.952  74.110  21.851  1.00115.56           C
ATOM    817  NE2 GLN C1014      16.046  74.585  22.709  1.00115.52           N
ATOM    818  OE1 GLN C1014      16.667  73.288  20.966  1.00116.95           O
ATOM    819  N   GLU C1015      17.510  73.830  25.926  1.00100.51           N
ATOM    820  CA  GLU C1015      16.178  73.788  26.534  1.00 95.53           C
ATOM    821  C   GLU C1015      15.959  74.945  27.489  1.00 90.60           C
ATOM    822  O   GLU C1015      15.087  75.788  27.249  1.00 84.83           O
ATOM    823  CB  GLU C1015      15.948  72.449  27.250  1.00 97.24           C
ATOM    824  CG  GLU C1015      14.516  72.235  27.763  1.00101.85           C
ATOM    825  CD  GLU C1015      13.407  72.502  26.710  1.00104.25           C
ATOM    826  OE1 GLU C1015      13.570  72.137  25.521  1.00100.17           O
ATOM    827  OE2 GLU C1015      12.350  73.065  27.091  1.00103.74
O1-
ATOM    828  N   TYR C1016      16.768  74.996  28.544  1.00 86.99           N
ATOM    829  CA  TYR C1016      16.673  76.060  29.532  1.00 90.23           C
ATOM    830  C   TYR C1016      16.819  77.464  28.935  1.00 91.23           C
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ATOM    831  O   TYR C1016      16.740  78.461  29.666  1.00 91.81           O
ATOM    832  CB  TYR C1016      17.702  75.847  30.649  1.00 92.03           C
ATOM    833  CG  TYR C1016      17.413  74.621  31.485  1.00 96.31           C
ATOM    834  CD1 TYR C1016      16.145  74.410  32.027  1.00 95.33           C
ATOM    835  CD2 TYR C1016      18.383  73.639  31.681  1.00 99.21           C
ATOM    836  CE1 TYR C1016      15.844  73.247  32.736  1.00 97.48           C
ATOM    837  CE2 TYR C1016      18.090  72.467  32.394  1.00 98.50           C
ATOM    838  CZ  TYR C1016      16.817  72.282  32.915  1.00 96.64           C
ATOM    839  OH  TYR C1016      16.513  71.138  33.617  1.00 95.40           O
ATOM    840  N   LYS C1017      17.041  77.543  27.622  1.00 90.88           N
ATOM    841  CA  LYS C1017      17.140  78.835  26.949  1.00 89.24           C
ATOM    842  C   LYS C1017      15.755  79.157  26.417  1.00 85.90           C
ATOM    843  O   LYS C1017      15.328  80.314  26.415  1.00 82.40           O
ATOM    844  CB  LYS C1017      18.142  78.810  25.787  1.00 93.74           C
ATOM    845  CG  LYS C1017      19.596  79.054  26.190  1.00 96.49           C
ATOM    846  CD  LYS C1017      20.433  79.517  24.996  1.00 96.88           C
ATOM    847  CE  LYS C1017      21.907  79.641  25.351  1.00 98.92           C
ATOM    848  NZ  LYS C1017      22.677  80.119  24.171  1.00100.42
N1+
ATOM    849  N   LYS C1018      15.055  78.131  25.949  1.00 83.14           N
ATOM    850  CA  LYS C1018      13.708  78.342  25.457  1.00 87.47           C
ATOM    851  C   LYS C1018      12.835  78.752  26.640  1.00 87.65           C
ATOM    852  O   LYS C1018      11.830  79.466  26.483  1.00 84.27           O
ATOM    853  CB  LYS C1018      13.169  77.070  24.822  1.00 89.97           C
ATOM    854  CG  LYS C1018      13.613  76.895  23.399  1.00 96.20           C
ATOM    855  CD  LYS C1018      12.885  75.739  22.745  1.00103.28           C
ATOM    856  CE  LYS C1018      13.303  75.560  21.291  1.00104.51           C
ATOM    857  NZ  LYS C1018      12.940  74.192  20.792  1.00103.98
N1+
ATOM    858  N   GLN C1019      13.241  78.285  27.822  1.00 85.24           N
ATOM    859  CA  GLN C1019      12.546  78.585  29.061  1.00 80.75           C
ATOM    860  C   GLN C1019      12.922  79.979  29.522  1.00 82.79           C
ATOM    861  O   GLN C1019      12.105  80.666  30.135  1.00 86.11           O
ATOM    862  CB  GLN C1019      12.873  77.535  30.125  1.00 74.33           C
ATOM    863  CG  GLN C1019      12.050  76.272  29.950  1.00 72.25           C
ATOM    864  CD  GLN C1019      12.450  75.178  30.917  1.00 73.41           C
ATOM    865  NE2 GLN C1019      12.486  73.935  30.434  1.00 77.00           N
ATOM    866  OE1 GLN C1019      12.715  75.442  32.088  1.00 72.63           O
ATOM    867  N   MET C1020      14.154  80.399  29.236  1.00 85.11           N
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ATOM    868  CA  MET C1020      14.577  81.749  29.591  1.00 84.66           C
ATOM    869  C   MET C1020      13.717  82.684  28.746  1.00 83.25           C
ATOM    870  O   MET C1020      13.164  83.656  29.247  1.00 83.62           O
ATOM    871  CB  MET C1020      16.067  81.966  29.285  1.00 85.31           C
ATOM    872  CG  MET C1020      16.959  81.858  30.524  1.00 90.41           C
ATOM    873  SD  MET C1020      18.753  81.804  30.222  1.00 91.63           S
ATOM    874  CE  MET C1020      19.239  83.527  30.360  1.00 88.91           C
ATOM    875  N   LEU C1021      13.587  82.377  27.462  1.00 80.01           N
ATOM    876  CA  LEU C1021      12.779  83.218  26.596  1.00 81.04           C
ATOM    877  C   LEU C1021      11.353  83.338  27.097  1.00 81.68           C
ATOM    878  O   LEU C1021      10.759  84.411  27.065  1.00 80.93           O
ATOM    879  CB  LEU C1021      12.737  82.661  25.179  1.00 84.04           C
ATOM    880  CG  LEU C1021      13.983  82.688  24.301  1.00 83.49           C
ATOM    881  CD1 LEU C1021      13.507  83.028  22.895  1.00 80.96           C
ATOM    882  CD2 LEU C1021      14.998  83.724  24.779  1.00 80.98           C
ATOM    883  N   THR C1022      10.811  82.207  27.531  1.00 84.90           N
ATOM    884  CA  THR C1022       9.446  82.110  28.037  1.00 85.69           C
ATOM    885  C   THR C1022       9.251  83.048  29.208  1.00 83.51           C
ATOM    886  O   THR C1022       8.390  83.934  29.197  1.00 80.07           O
ATOM    887  CB  THR C1022       9.154  80.637  28.469  1.00 88.46           C
ATOM    888  CG2 THR C1022       8.259  80.570  29.712  1.00 90.20           C
ATOM    889  OG1 THR C1022       8.543  79.941  27.374  1.00 91.00           O
ATOM    890  N   ALA C1023      10.092  82.826  30.208  1.00 81.70           N
ATOM    891  CA  ALA C1023      10.094  83.586  31.436  1.00 83.77           C
ATOM    892  C   ALA C1023      10.250  85.077  31.213  1.00 85.16           C
ATOM    893  O   ALA C1023       9.714  85.859  31.998  1.00 89.04           O
ATOM    894  CB  ALA C1023      11.210  83.085  32.352  1.00 83.59           C
ATOM    895  N   ALA C1024      10.980  85.470  30.163  1.00 81.68           N
ATOM    896  CA  ALA C1024      11.214  86.887  29.875  1.00 75.41           C
ATOM    897  C   ALA C1024      10.025  87.513  29.145  1.00 73.27           C
ATOM    898  O   ALA C1024       9.701  88.680  29.359  1.00 72.93           O
ATOM    899  CB  ALA C1024      12.501  87.061  29.070  1.00 65.77           C
ATOM    900  N   HIS C1025       9.369  86.740  28.290  1.00 68.05           N
ATOM    901  CA  HIS C1025       8.209  87.249  27.576  1.00 68.21           C
ATOM    902  C   HIS C1025       7.117  87.527  28.621  1.00 69.52           C
ATOM    903  O   HIS C1025       6.305  88.444  28.459  1.00 65.51           O
ATOM    904  CB  HIS C1025       7.727  86.206  26.551  1.00 71.98           C
ATOM    905  CG  HIS C1025       6.534  86.631  25.743  1.00 78.78           C
ATOM    906  CD2 HIS C1025       6.449  87.173  24.501  1.00 83.90           C
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ATOM    907  ND1 HIS C1025       5.237  86.520  26.198  1.00 84.22           N
ATOM    908  CE1 HIS C1025       4.406  86.975  25.277  1.00 87.90           C
ATOM    909  NE2 HIS C1025       5.113  87.378  24.237  1.00 86.95           N
ATOM    910  N   ALA C1026       7.119  86.732  29.696  1.00 68.89           N
ATOM    911  CA  ALA C1026       6.127  86.843  30.766  1.00 66.22           C
ATOM    912  C   ALA C1026       6.342  88.146  31.470  1.00 67.21           C
ATOM    913  O   ALA C1026       5.411  88.917  31.693  1.00 70.82           O
ATOM    914  CB  ALA C1026       6.289  85.720  31.729  1.00 59.99           C
ATOM    915  N   LEU C1027       7.594  88.373  31.826  1.00 65.47           N
ATOM    916  CA  LEU C1027       7.994  89.597  32.467  1.00 63.68           C
ATOM    917  C   LEU C1027       7.507  90.779  31.624  1.00 64.67           C
ATOM    918  O   LEU C1027       7.048  91.774  32.164  1.00 70.41           O
ATOM    919  CB  LEU C1027       9.516  89.625  32.591  1.00 60.17           C
ATOM    920  CG  LEU C1027      10.140  90.845  33.254  1.00 61.80           C
ATOM    921  CD1 LEU C1027       9.381  91.159  34.512  1.00 64.53           C
ATOM    922  CD2 LEU C1027      11.599  90.582  33.579  1.00 66.87           C
ATOM    923  N   ALA C1028       7.577  90.669  30.302  1.00 62.81           N
ATOM    924  CA  ALA C1028       7.152  91.773  29.448  1.00 63.80           C
ATOM    925  C   ALA C1028       5.645  91.975  29.356  1.00 64.53           C
ATOM    926  O   ALA C1028       5.173  93.107  29.348  1.00 63.07           O
ATOM    927  CB  ALA C1028       7.717  91.600  28.068  1.00 62.94           C
ATOM    928  N   VAL C1029       4.890  90.887  29.265  1.00 66.59           N
ATOM    929  CA  VAL C1029       3.439  90.986  29.172  1.00 67.48           C
ATOM    930  C   VAL C1029       2.884  91.582  30.461  1.00 67.97           C
ATOM    931  O   VAL C1029       1.915  92.351  30.448  1.00 65.88           O
ATOM    932  CB  VAL C1029       2.824  89.607  28.930  1.00 66.88           C
ATOM    933  CG1 VAL C1029       1.330  89.730  28.727  1.00 63.81           C
ATOM    934  CG2 VAL C1029       3.472  88.985  27.709  1.00 66.42           C
ATOM    935  N   ASP C1030       3.521  91.222  31.570  1.00 65.23           N
ATOM    936  CA  ASP C1030       3.126  91.712  32.880  1.00 64.94           C
ATOM    937  C   ASP C1030       3.488  93.173  33.094  1.00 62.44           C
ATOM    938  O   ASP C1030       2.701  93.927  33.658  1.00 64.35           O
ATOM    939  CB  ASP C1030       3.735  90.839  33.992  1.00 65.96           C
ATOM    940  CG  ASP C1030       2.911  89.578  34.255  1.00 69.57           C
ATOM    941  OD1 ASP C1030       1.701  89.591  33.944  1.00 67.28           O
ATOM    942  OD2 ASP C1030       3.454  88.585  34.783  1.00 71.94
O1-
ATOM    943  N   ALA C1031       4.668  93.576  32.643  1.00 59.88           N
ATOM    944  CA  ALA C1031       5.072  94.959  32.796  1.00 57.53           C
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ATOM    945  C   ALA C1031       4.022  95.837  32.109  1.00 59.49           C
ATOM    946  O   ALA C1031       3.706  96.935  32.579  1.00 58.64           O
ATOM    947  CB  ALA C1031       6.428  95.162  32.176  1.00 51.37           C
ATOM    948  N   LYS C1032       3.470  95.345  31.002  1.00 59.00           N
ATOM    949  CA  LYS C1032       2.466  96.094  30.270  1.00 57.05           C
ATOM    950  C   LYS C1032       1.148  96.057  31.023  1.00 60.38           C
ATOM    951  O   LYS C1032       0.296  96.936  30.854  1.00 57.03           O
ATOM    952  CB  LYS C1032       2.309  95.513  28.862  1.00 56.79           C
ATOM    953  CG  LYS C1032       3.458  95.897  27.918  1.00 62.37           C
ATOM    954  CD  LYS C1032       3.612  94.970  26.703  1.00 68.50           C
ATOM    955  CE  LYS C1032       2.945  95.535  25.447  1.00 72.18           C
ATOM    956  NZ  LYS C1032       3.085  94.605  24.287  1.00 75.66
N1+
ATOM    957  N   ASN C1033       0.971  95.031  31.855  1.00 63.06           N
ATOM    958  CA  ASN C1033      -0.264  94.919  32.623  1.00 62.59           C
ATOM    959  C   ASN C1033      -0.163  95.835  33.817  1.00 59.41           C
ATOM    960  O   ASN C1033      -1.151  96.441  34.210  1.00 57.40           O
ATOM    961  CB  ASN C1033      -0.530  93.471  33.044  1.00 64.82           C
ATOM    962  CG  ASN C1033      -1.004  92.614  31.880  1.00 74.38           C
ATOM    963  ND2 ASN C1033      -1.214  93.253  30.728  1.00 79.97           N
ATOM    964  OD1 ASN C1033      -1.185  91.398  32.009  1.00 78.02           O
ATOM    965  N   LEU C1034       1.039  95.945  34.375  1.00 56.92           N
ATOM    966  CA  LEU C1034       1.276  96.829  35.495  1.00 55.84           C
ATOM    967  C   LEU C1034       0.805  98.193  35.032  1.00 59.67           C
ATOM    968  O   LEU C1034      -0.033  98.835  35.671  1.00 65.25           O
ATOM    969  CB  LEU C1034       2.760  96.887  35.807  1.00 56.08           C
ATOM    970  CG  LEU C1034       3.112  97.924  36.866  1.00 64.48           C
ATOM    971  CD1 LEU C1034       2.306  97.609  38.101  1.00 67.21           C
ATOM    972  CD2 LEU C1034       4.603  97.907  37.181  1.00 64.72           C
ATOM    973  N   LEU C1035       1.357  98.626  33.903  1.00 58.09           N
ATOM    974  CA  LEU C1035       1.020  99.901  33.296  1.00 55.87           C
ATOM    975  C   LEU C1035      -0.486 100.027  33.167  1.00 51.30           C
ATOM    976  O   LEU C1035      -1.049 101.029  33.547  1.00 48.73           O
ATOM    977  CB  LEU C1035       1.658  99.996  31.916  1.00 58.28           C
ATOM    978  CG  LEU C1035       1.914 101.349  31.273  1.00 59.39           C
ATOM    979  CD1 LEU C1035       2.086 101.110  29.799  1.00 59.31           C
ATOM    980  CD2 LEU C1035       0.767 102.299  31.500  1.00 62.27           C
ATOM    981  N   ASP C1036      -1.143  99.014  32.622  1.00 53.83           N
ATOM    982  CA  ASP C1036      -2.592  99.079  32.488  1.00 58.81           C
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ATOM    983  C   ASP C1036      -3.343  99.361  33.809  1.00 60.83           C
ATOM    984  O   ASP C1036      -4.246 100.197  33.825  1.00 58.01           O
ATOM    985  CB  ASP C1036      -3.127  97.802  31.862  1.00 63.90           C
ATOM    986  CG  ASP C1036      -4.650  97.795  31.771  1.00 75.23           C
ATOM    987  OD1 ASP C1036      -5.274  96.953  32.452  1.00 86.78           O
ATOM    988  OD2 ASP C1036      -5.224  98.627  31.032  1.00 80.05
O1-
ATOM    989  N   VAL C1037      -2.998  98.656  34.892  1.00 63.64           N
ATOM    990  CA  VAL C1037      -3.616  98.860  36.209  1.00 63.82           C
ATOM    991  C   VAL C1037      -3.492 100.351  36.588  1.00 65.23           C
ATOM    992  O   VAL C1037      -4.497 101.060  36.788  1.00 68.35           O
ATOM    993  CB  VAL C1037      -2.887  98.017  37.278  1.00 65.81           C
ATOM    994  CG1 VAL C1037      -3.460  98.265  38.655  1.00 63.68           C
ATOM    995  CG2 VAL C1037      -3.008  96.576  36.932  1.00 66.00           C
ATOM    996  N   ILE C1038      -2.254 100.830  36.684  1.00 56.67           N
ATOM    997  CA  ILE C1038      -1.988 102.232  37.008  1.00 52.09           C
ATOM    998  C   ILE C1038      -2.795 103.253  36.154  1.00 56.52           C
ATOM    999  O   ILE C1038      -3.207 104.319  36.643  1.00 61.00           O
ATOM   1000  CB  ILE C1038      -0.506 102.495  36.857  1.00 40.92           C
ATOM   1001  CG1 ILE C1038       0.251 101.813  37.991  1.00 40.83           C
ATOM   1002  CG2 ILE C1038      -0.241 103.944  36.878  1.00 44.37           C
ATOM   1003  CD1 ILE C1038       1.781 101.856  37.871  1.00 43.08           C
ATOM   1004  N   ASP C1039      -3.016 102.951  34.880  1.00 58.87           N
ATOM   1005  CA  ASP C1039      -3.788 103.863  34.044  1.00 63.24           C
ATOM   1006  C   ASP C1039      -5.223 103.847  34.553  1.00 62.31           C
ATOM   1007  O   ASP C1039      -5.846 104.903  34.639  1.00 61.21           O
ATOM   1008  CB  ASP C1039      -3.712 103.478  32.540  1.00 64.64           C
ATOM   1009  CG  ASP C1039      -2.406 103.983  31.850  1.00 70.50           C
ATOM   1010  OD1 ASP C1039      -1.519 104.598  32.524  1.00 64.94           O
ATOM   1011  OD2 ASP C1039      -2.283 103.749  30.621  1.00 73.26
O1-
ATOM   1012  N   GLN C1040      -5.755 102.667  34.885  1.00 63.31           N
ATOM   1013  CA  GLN C1040      -7.122 102.585  35.423  1.00 66.22           C
ATOM   1014  C   GLN C1040      -7.111 103.430  36.720  1.00 65.53           C
ATOM   1015  O   GLN C1040      -8.056 104.175  37.036  1.00 57.11           O
ATOM   1016  CB  GLN C1040      -7.481 101.143  35.783  1.00 69.30           C
ATOM   1017  CG  GLN C1040      -7.457 100.156  34.667  1.00 80.10           C
ATOM   1018  CD  GLN C1040      -7.681  98.738  35.175  1.00 87.83           C
ATOM   1019  NE2 GLN C1040      -6.715  97.844  34.925  1.00 91.51           N
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ATOM   1020  OE1 GLN C1040      -8.711  98.452  35.790  1.00 91.10           O
ATOM   1021  N   ALA C1041      -6.022 103.283  37.469  1.00 62.66           N
ATOM   1022  CA  ALA C1041      -5.853 104.025  38.698  1.00 62.47           C
ATOM   1023  C   ALA C1041      -5.868 105.525  38.400  1.00 66.44           C
ATOM   1024  O   ALA C1041      -6.569 106.275  39.088  1.00 69.97           O
ATOM   1025  CB  ALA C1041      -4.539 103.635  39.384  1.00 59.49           C
ATOM   1026  N   ARG C1042      -5.125 105.994  37.398  1.00 65.45           N
ATOM   1027  CA  ARG C1042      -5.170 107.435  37.161  1.00 67.91           C
ATOM   1028  C   ARG C1042      -6.545 107.875  36.667  1.00 68.21           C
ATOM   1029  O   ARG C1042      -7.045 108.920  37.077  1.00 67.77           O
ATOM   1030  CB  ARG C1042      -4.091 107.883  36.179  1.00 63.15           C
ATOM   1031  CG  ARG C1042      -2.707 107.699  36.725  1.00 64.59           C
ATOM   1032  CD  ARG C1042      -1.821 107.089  35.661  1.00 64.74           C
ATOM   1033  NE  ARG C1042      -0.396 107.291  35.918  1.00 58.12           N
ATOM   1034  CZ  ARG C1042       0.562 107.019  35.038  1.00 55.70           C
ATOM   1035  NH1 ARG C1042       0.252 106.537  33.842  1.00 57.33
N1+
ATOM   1036  NH2 ARG C1042       1.829 107.216  35.350  1.00 49.95           N
ATOM   1037  N   LEU C1043      -7.161 107.079  35.801  1.00 68.03           N
ATOM   1038  CA  LEU C1043      -8.468 107.436  35.285  1.00 73.06           C
ATOM   1039  C   LEU C1043      -9.472 107.546  36.432  1.00 78.30           C
ATOM   1040  O   LEU C1043     -10.299 108.463  36.451  1.00 77.88           O
ATOM   1041  CB  LEU C1043      -8.927 106.404  34.246  1.00 69.68           C
ATOM   1042  CG  LEU C1043      -8.057 106.338  32.978  1.00 69.22           C
ATOM   1043  CD1 LEU C1043      -8.528 105.195  32.108  1.00 66.15           C
ATOM   1044  CD2 LEU C1043      -8.101 107.653  32.205  1.00 62.85           C
ATOM   1045  N   LYS C1044      -9.389 106.622  37.393  1.00 83.18           N
ATOM   1046  CA  LYS C1044     -10.296 106.640  38.539  1.00 84.86           C
ATOM   1047  C   LYS C1044     -10.144 107.999  39.194  1.00 85.31           C
ATOM   1048  O   LYS C1044     -11.125 108.673  39.520  1.00 85.59           O
ATOM   1049  CB  LYS C1044      -9.934 105.558  39.566  1.00 85.94           C
ATOM   1050  CG  LYS C1044     -11.166 104.960  40.237  1.00 91.52           C
ATOM   1051  CD  LYS C1044     -10.911 104.331  41.601  1.00 91.04           C
ATOM   1052  CE  LYS C1044     -12.193 103.660  42.097  1.00 90.64           C
ATOM   1053  NZ  LYS C1044     -12.051 103.064  43.449  1.00 91.14
N1+
ATOM   1054  N   MET C1045      -8.795 108.526  39.447  1.00  0.00           N
ATOM   1055  CA  MET C1045      -8.977 109.831  40.076  1.00  0.00           C
ATOM   1056  C   MET C1045      -9.807 110.743  39.205  1.00  0.00           C
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ATOM   1057  O   MET C1045      -9.606 110.845  37.985  1.00  0.00           O
ATOM   1058  CB  MET C1045      -7.592 110.466  40.382  1.00  0.00           C
ATOM   1059  CG  MET C1045      -6.702 109.693  41.379  1.00  0.00           C
ATOM   1060  SD  MET C1045      -5.283 110.701  41.838  1.00  0.00           S
ATOM   1061  CE  MET C1045      -4.298 109.426  42.635  1.00  0.00           C
ATOM   1062  H   MET C1045      -7.857 108.044  39.214  1.00  0.00           H
ATOM   1063  HA  MET C1045      -9.533 109.692  41.022  1.00  0.00           H
ATOM   1064 2HB  MET C1045      -7.739 111.487  40.784  1.00  0.00           H
ATOM   1065 3HB  MET C1045      -7.028 110.611  39.439  1.00  0.00           H
ATOM   1066 2HG  MET C1045      -6.348 108.751  40.919  1.00  0.00           H
ATOM   1067 3HG  MET C1045      -7.260 109.412  42.291  1.00  0.00           H
ATOM   1068 1HE  MET C1045      -4.864 108.940  43.450  1.00  0.00           H
ATOM   1069 2HE  MET C1045      -4.005 108.652  41.904  1.00  0.00           H
ATOM   1070 3HE  MET C1045      -3.377 109.860  43.063  1.00  0.00           H
ATOM   1071  N   LEU C1046     -10.884 111.532  39.820  1.00  0.00           N
ATOM   1072  CA  LEU C1046     -11.494 112.302  38.740  1.00  0.00           C
ATOM   1073  C   LEU C1046     -11.807 113.709  39.190  1.00  0.00           C
ATOM   1074  O   LEU C1046     -12.669 113.948  40.049  1.00  0.00           O
ATOM   1075  CB  LEU C1046     -12.774 111.589  38.217  1.00  0.00           C
ATOM   1076  CG  LEU C1046     -12.634 110.138  37.680  1.00  0.00           C
ATOM   1077  CD1 LEU C1046     -13.975 109.654  37.111  1.00  0.00           C
ATOM   1078  CD2 LEU C1046     -11.538 110.003  36.610  1.00  0.00           C
ATOM   1079  H   LEU C1046     -11.152 111.540  40.809  1.00  0.00           H
ATOM   1080  HA  LEU C1046     -10.761 112.395  37.919  1.00  0.00           H
ATOM   1081 2HB  LEU C1046     -13.221 112.212  37.418  1.00  0.00           H
ATOM   1082 3HB  LEU C1046     -13.533 111.585  39.024  1.00  0.00           H
ATOM   1083  HG  LEU C1046     -12.368 109.479  38.533  1.00  0.00           H
ATOM   1084 1HD1 LEU C1046     -14.782 109.696  37.867  1.00  0.00           H
ATOM   1085 2HD1 LEU C1046     -14.306 110.260  36.246  1.00  0.00           H
ATOM   1086 3HD1 LEU C1046     -13.917 108.604  36.770  1.00  0.00           H
ATOM   1087 1HD2 LEU C1046     -11.696 110.691  35.760  1.00  0.00           H
ATOM   1088 2HD2 LEU C1046     -10.538 110.223  37.030  1.00  0.00           H
ATOM   1089 3HD2 LEU C1046     -11.479 108.976  36.205  1.00  0.00           H
ATOM   1090  N   GLY C1047     -11.068 114.829  38.591  1.00  0.00           N
ATOM   1091  CA  GLY C1047     -11.584 116.042  39.218  1.00  0.00           C
ATOM   1092  C   GLY C1047     -12.201 116.961  38.191  1.00  0.00           C
ATOM   1093  O   GLY C1047     -13.305 117.486  38.363  1.00  0.00           O
ATOM   1094  H   GLY C1047     -10.296 114.767  37.838  1.00  0.00           H
ATOM   1095 3HA  GLY C1047     -10.786 116.535  39.690  0.00  0.00           H
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ATOM   1096  HA  GLY C1047     -12.372 115.764  39.943  1.00  0.00           H
ATOM   1097  N   GLN C1048     -11.466 117.237  36.949  1.00  0.00           N
ATOM   1098  CA  GLN C1048     -12.304 118.142  36.169  1.00  0.00           C
ATOM   1099  C   GLN C1048     -13.667 117.540  35.920  1.00  0.00           C
ATOM   1100  O   GLN C1048     -13.807 116.372  35.565  1.00  0.00           O
ATOM   1101  CB  GLN C1048     -11.587 118.459  34.838  1.00  0.00           C
ATOM   1102  CG  GLN C1048     -12.317 119.458  33.881  1.00  0.00           C
ATOM   1103  CD  GLN C1048     -11.695 119.772  32.514  1.00  0.00           C
ATOM   1104  NE2 GLN C1048     -10.560 119.220  32.169  1.00  0.00           N
ATOM   1105  OE1 GLN C1048     -12.254 120.516  31.723  1.00  0.00           O
ATOM   1106  H   GLN C1048     -10.605 116.891  36.700  1.00  0.00           H
ATOM   1107  HA  GLN C1048     -12.451 119.075  36.745  1.00  0.00           H
ATOM   1108 2HB  GLN C1048     -11.411 117.506  34.297  1.00  0.00           H
ATOM   1109 3HB  GLN C1048     -10.578 118.858  35.060  1.00  0.00           H
ATOM   1110 2HG  GLN C1048     -12.489 120.421  34.396  1.00  0.00           H
ATOM   1111 3HG  GLN C1048     -13.332 119.090  33.643  1.00  0.00           H
ATOM   1112 1HE2 GLN C1048     -10.248 119.431  31.220  1.00  0.00           H
ATOM   1113 2HE2 GLN C1048     -10.180 118.556  32.846  1.00  0.00           H
ATOM   1114  N   MET C1049     -14.861 118.377  36.108  1.00  0.00           N
ATOM   1115  CA  MET C1049     -16.008 117.529  35.797  1.00  0.00           C
ATOM   1116  C   MET C1049     -17.045 118.288  35.005  1.00  0.00           C
ATOM   1117  O   MET C1049     -17.685 119.231  35.495  1.00  0.00           O
ATOM   1118  CB  MET C1049     -16.618 116.964  37.110  1.00  0.00           C
ATOM   1119  CG  MET C1049     -15.695 116.050  37.943  1.00  0.00           C
ATOM   1120  SD  MET C1049     -16.641 115.260  39.256  1.00  0.00           S
ATOM   1121  CE  MET C1049     -15.269 114.628  40.229  1.00  0.00           C
ATOM   1122  H   MET C1049     -14.885 119.412  36.415  1.00  0.00           H
ATOM   1123  HA  MET C1049     -15.665 116.690  35.163  1.00  0.00           H
ATOM   1124 2HB  MET C1049     -17.533 116.390  36.871  1.00  0.00           H
ATOM   1125 3HB  MET C1049     -16.967 117.798  37.752  1.00  0.00           H
ATOM   1126 2HG  MET C1049     -14.875 116.644  38.389  1.00  0.00           H
ATOM   1127 3HG  MET C1049     -15.219 115.272  37.318  1.00  0.00           H
ATOM   1128 1HE  MET C1049     -14.611 113.985  39.616  1.00  0.00           H
ATOM   1129 2HE  MET C1049     -14.666 115.461  40.631  1.00  0.00           H
ATOM   1130 3HE  MET C1049     -15.641 114.031  41.080  1.00  0.00           H
ATOM   1131  N   ARG C1050     -17.302 117.900  33.610  1.00  0.00           N
ATOM   1132  CA  ARG C1050     -18.338 118.804  33.118  1.00  0.00           C
ATOM   1133  C   ARG C1050     -19.573 118.038  32.708  1.00  0.00           C
ATOM   1134  O   ARG C1050     -19.576 117.273  31.746  1.00  0.00           O
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ATOM   1135  CB  ARG C1050     -17.762 119.628  31.932  1.00  0.00           C
ATOM   1136  CG  ARG C1050     -18.633 120.829  31.466  1.00  0.00           C
ATOM   1137  CD  ARG C1050     -18.009 121.565  30.269  1.00  0.00           C
ATOM   1138  NE  ARG C1050     -18.876 122.716  29.881  1.00  0.00           N
ATOM   1139  CZ  ARG C1050     -18.633 123.558  28.880  1.00  0.00           C
ATOM   1140  NH1 ARG C1050     -17.592 123.472  28.101  1.00  0.00
N1+
ATOM   1141  NH2 ARG C1050     -19.476 124.518  28.666  1.00  0.00           N
ATOM   1142  H   ARG C1050     -16.845 117.145  33.087  1.00  0.00           H
ATOM   1143  HA  ARG C1050     -18.623 119.480  33.947  1.00  0.00           H
ATOM   1144 2HB  ARG C1050     -17.573 118.942  31.080  1.00  0.00           H
ATOM   1145 3HB  ARG C1050     -16.756 120.007  32.207  1.00  0.00           H
ATOM   1146 2HG  ARG C1050     -18.779 121.525  32.317  1.00  0.00           H
ATOM   1147 3HG  ARG C1050     -19.648 120.477  31.190  1.00  0.00           H
ATOM   1148 2HD  ARG C1050     -17.889 120.855  29.422  1.00  0.00           H
ATOM   1149 3HD  ARG C1050     -16.987 121.909  30.537  1.00  0.00           H
ATOM   1150  HE  ARG C1050     -19.739 122.924  30.393  1.00  0.00           H
ATOM   1151 1HH1 ARG C1050     -16.968 122.693  28.323  1.00  0.00           H
ATOM   1152 2HH1 ARG C1050     -17.476 124.159  27.354  1.00  0.00           H
ATOM   1153 1HH2 ARG C1050     -20.287 124.569  29.286  1.00  0.00           H
ATOM   1154 2HH2 ARG C1050     -19.272 125.155  27.894  1.00  0.00           H
ATOM   1155  N   PRO C1051     -20.810 118.212  33.483  1.00  0.00           N
ATOM   1156  CA  PRO C1051     -21.839 117.372  32.888  1.00  0.00           C
ATOM   1157  C   PRO C1051     -21.398 116.818  31.523  1.00  0.00           C
ATOM   1158  O   PRO C1051     -21.240 117.574  30.564  1.00  0.00           O
ATOM   1159  CB  PRO C1051     -23.022 118.346  32.787  1.00  0.00           C
ATOM   1160  CG  PRO C1051     -22.350 119.716  32.614  1.00  0.00           C
ATOM   1161  CD  PRO C1051     -21.122 119.624  33.523  1.00  0.00           C
ATOM   1162  HA  PRO C1051     -22.078 116.534  33.547  1.00  0.00           H
ATOM   1163 2HB  PRO C1051     -23.575 118.333  33.729  1.00  0.00           H
ATOM   1164 3HB  PRO C1051     -23.705 118.103  31.970  1.00  0.00           H
ATOM   1165 2HG  PRO C1051     -23.007 120.544  32.892  1.00  0.00           H
ATOM   1166 3HG  PRO C1051     -22.028 119.838  31.578  1.00  0.00           H
ATOM   1167 2HD  PRO C1051     -21.369 119.915  34.546  1.00  0.00           H
ATOM   1168 3HD  PRO C1051     -20.287 120.222  33.150  1.00  0.00           H
ATOM   1169  N   HIS C1052     -21.164 115.375  31.362  1.00  0.00           N
ATOM   1170  CA  HIS C1052     -20.764 115.178  29.971  1.00  0.00           C
ATOM   1171  C   HIS C1052     -21.737 114.277  29.250  1.00  0.00           C
ATOM   1172  O   HIS C1052     -22.730 113.795  29.816  1.00  0.00           O
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ATOM   1173  CB  HIS C1052     -19.367 114.536  30.011  1.00  0.00           C
ATOM   1174  CG  HIS C1052     -18.330 115.386  29.337  1.00  0.00           C
ATOM   1175  CD2 HIS C1052     -17.584 116.339  30.017  1.00  0.00           C
ATOM   1176  ND1 HIS C1052     -17.985 115.337  27.988  1.00  0.00           N
ATOM   1177  CE1 HIS C1052     -17.038 116.292  27.957  1.00  0.00           C
ATOM   1178  NE2 HIS C1052     -16.737 116.934  29.118  1.00  0.00           N
ATOM   1179  H   HIS C1052     -21.268 114.614  32.120  1.00  0.00           H
ATOM   1180  HA  HIS C1052     -20.809 116.158  29.468  1.00  0.00           H
ATOM   1181 2HB  HIS C1052     -19.368 113.544  29.517  1.00  0.00           H
ATOM   1182 3HB  HIS C1052     -19.023 114.346  31.049  1.00  0.00           H
ATOM   1183 2HD  HIS C1052     -17.679 116.553  31.078  1.00  0.00           H
ATOM   1184 1HE  HIS C1052     -16.563 116.496  27.007  1.00  0.00           H
ATOM   1185 2HE  HIS C1052     -16.049 117.682  29.288  1.00  0.00           H
TER    1186      HIS C1052
ATOM   1187  N   SER D  -3      -7.859 112.514  13.714  1.00  0.00           N
ATOM   1188  CA  SER D  -3      -7.673 111.506  14.754  1.00  0.00           C
ATOM   1189  C   SER D  -3      -6.214 111.371  15.121  1.00  0.00           C
ATOM   1190  O   SER D  -3      -5.330 111.314  14.267  1.00  0.00           O
ATOM   1191  CB  SER D  -3      -8.280 110.148  14.321  1.00  0.00           C
ATOM   1192  OG  SER D  -3      -7.550 109.526  13.258  1.00  0.00           O
ATOM   1193  H   SER D  -3      -7.031 113.064  13.294  1.00  0.00           H
ATOM   1194  HA  SER D  -3      -8.201 111.852  15.662  1.00  0.00           H
ATOM   1195 2HB  SER D  -3      -9.340 110.260  14.025  1.00  0.00           H
ATOM   1196 3HB  SER D  -3      -8.296 109.455  15.185  1.00  0.00           H
ATOM   1197  HG  SER D  -3      -7.607 110.105  12.494  1.00  0.00           H
ATOM   1198  N   ALA D  -2      -5.839 111.306  16.541  1.00  0.00           N
ATOM   1199  CA  ALA D  -2      -4.385 111.179  16.575  1.00  0.00           C
ATOM   1200  C   ALA D  -2      -3.954 110.189  17.630  1.00  0.00           C
ATOM   1201  O   ALA D  -2      -4.439 110.189  18.768  1.00  0.00           O
ATOM   1202  CB  ALA D  -2      -3.799 112.584  16.801  1.00  0.00           C
ATOM   1203  H   ALA D  -2      -6.506 111.345  17.390  1.00  0.00           H
ATOM   1204  HA  ALA D  -2      -4.041 110.790  15.599  1.00  0.00           H
ATOM   1205 1HB  ALA D  -2      -4.095 113.286  15.998  1.00  0.00           H
ATOM   1206 2HB  ALA D  -2      -4.136 113.027  17.758  1.00  0.00           H
ATOM   1207 3HB  ALA D  -2      -2.694 112.571  16.819  1.00  0.00           H
ATOM   1208  N   SER D  -1      -2.924 109.195  17.295  1.00  0.00           N
ATOM   1209  CA  SER D  -1      -2.723 108.392  18.498  1.00  0.00           C
ATOM   1210  C   SER D  -1      -1.257 108.102  18.716  1.00  0.00           C
ATOM   1211  O   SER D  -1      -0.521 107.740  17.799  1.00  0.00           O
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ATOM   1212  CB  SER D  -1      -3.559 107.089  18.438  1.00  0.00           C
ATOM   1213  OG  SER D  -1      -3.079 106.165  17.456  1.00  0.00           O
ATOM   1214  H   SER D  -1      -2.418 109.080  16.348  1.00  0.00           H
ATOM   1215  HA  SER D  -1      -3.065 108.987  19.366  1.00  0.00           H
ATOM   1216 2HB  SER D  -1      -4.627 107.307  18.248  1.00  0.00           H
ATOM   1217 3HB  SER D  -1      -3.541 106.589  19.426  1.00  0.00           H
ATOM   1218  HG  SER D  -1      -3.169 106.585  16.597  1.00  0.00           H
ATOM   1219  N   SER D   0      -0.692 108.257  20.065  1.00  0.00           N
ATOM   1220  CA  SER D   0       0.722 107.910  19.958  1.00  0.00           C
ATOM   1221  C   SER D   0       1.168 107.088  21.145  1.00  0.00           C
ATOM   1222  O   SER D   0       1.834 106.062  21.013  1.00  0.00           O
ATOM   1223  CB  SER D   0       1.590 109.182  19.787  1.00  0.00           C
ATOM   1224  OG  SER D   0       1.634 109.989  20.969  1.00  0.00           O
ATOM   1225  H   SER D   0      -1.218 108.565  20.956  1.00  0.00           H
ATOM   1226  HA  SER D   0       0.851 107.275  19.062  1.00  0.00           H
ATOM   1227 2HB  SER D   0       1.239 109.794  18.935  1.00  0.00           H
ATOM   1228 3HB  SER D   0       2.626 108.893  19.524  1.00  0.00           H
ATOM   1229  HG  SER D   0       0.740 110.292  21.143  1.00  0.00           H
ATOM   1230  N   ALA D   1       0.796 107.528  22.497  1.00  0.00           N
ATOM   1231  CA  ALA D   1       1.363 106.546  23.417  1.00  0.00           C
ATOM   1232  C   ALA D   1       0.867 105.156  23.096  1.00  0.00           C
ATOM   1233  O   ALA D   1       0.093 104.936  22.157  1.00  0.00           O
ATOM   1234  CB  ALA D   1       1.010 106.989  24.848  1.00  0.00           C
ATOM   1235  H   ALA D   1       0.219 108.403  22.758  1.00  0.00           H
ATOM   1236  HA  ALA D   1       2.462 106.540  23.294  1.00  0.00           H
ATOM   1237 1HB  ALA D   1       1.413 107.994  25.077  1.00  0.00           H
ATOM   1238 2HB  ALA D   1      -0.084 107.035  25.012  1.00  0.00           H
ATOM   1239 3HB  ALA D   1       1.424 106.300  25.606  1.00  0.00           H
ATOM   1240  N   THR D   2       1.264 104.168  23.824  1.00117.75           N
ATOM   1241  CA  THR D   2       1.121 102.693  23.972  1.00119.14           C
ATOM   1242  C   THR D   2       0.948 102.019  22.616  1.00120.27           C
ATOM   1243  O   THR D   2       0.822 100.802  22.543  1.00120.61           O
ATOM   1244  CB  THR D   2      -0.072 102.329  24.931  1.00119.19           C
ATOM   1245  CG2 THR D   2      -0.381 100.832  24.916  1.00114.83           C
ATOM   1246  OG1 THR D   2       0.278 102.693  26.273  1.00119.79           O
ATOM   1247  N   ARG D   3       0.943 102.794  21.534  1.00122.00           N
ATOM   1248  CA  ARG D   3       0.821 102.183  20.212  1.00122.43           C
ATOM   1249  C   ARG D   3       2.247 101.762  19.825  1.00121.24           C
ATOM   1250  O   ARG D   3       2.438 100.766  19.122  1.00120.23           O
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ATOM   1251  CB  ARG D   3       0.221 103.170  19.188  1.00124.89           C
ATOM   1252  CG  ARG D   3      -0.729 102.504  18.181  1.00127.61           C
ATOM   1253  CD  ARG D   3      -1.341 103.504  17.189  1.00131.95           C
ATOM   1254  NE  ARG D   3      -2.370 104.358  17.787  1.00136.27           N
ATOM   1255  CZ  ARG D   3      -3.151 105.196  17.101  1.00137.27           C
ATOM   1256  NH1 ARG D   3      -3.027 105.302  15.783  1.00136.09
N1+
ATOM   1257  NH2 ARG D   3      -4.065 105.926  17.729  1.00137.17           N
ATOM   1258  N   GLU D   4       3.236 102.515  20.322  1.00119.46           N
ATOM   1259  CA  GLU D   4       4.656 102.241  20.083  1.00117.02           C
ATOM   1260  C   GLU D   4       5.127 101.124  21.033  1.00113.77           C
ATOM   1261  O   GLU D   4       5.979 100.304  20.676  1.00112.68           O
ATOM   1262  CB  GLU D   4       5.479 103.524  20.283  1.00120.10           C
ATOM   1263  CG  GLU D   4       4.987 104.663  19.391  1.00125.95           C
ATOM   1264  CD  GLU D   4       6.071 105.680  19.009  1.00129.44           C
ATOM   1265  OE1 GLU D   4       6.490 106.502  19.860  1.00131.18           O
ATOM   1266  OE2 GLU D   4       6.509 105.652  17.839  1.00131.54
O1-
ATOM   1267  N   LEU D   5       4.576 101.115  22.247  1.00107.77           N
ATOM   1268  CA  LEU D   5       4.866 100.080  23.238  1.00100.20           C
ATOM   1269  C   LEU D   5       4.172  98.789  22.748  1.00101.89           C
ATOM   1270  O   LEU D   5       4.540  97.680  23.140  1.00103.23           O
ATOM   1271  CB  LEU D   5       4.292 100.486  24.607  1.00 89.57           C
ATOM   1272  CG  LEU D   5       4.171  99.393  25.678  1.00 82.95           C
ATOM   1273  CD1 LEU D   5       5.536  99.024  26.172  1.00 79.39           C
ATOM   1274  CD2 LEU D   5       3.338  99.860  26.837  1.00 78.40           C
ATOM   1275  N   ASP D   6       3.160  98.945  21.894  1.00103.15           N
ATOM   1276  CA  ASP D   6       2.414  97.808  21.365  1.00104.18           C
ATOM   1277  C   ASP D   6       3.096  97.197  20.153  1.00103.81           C
ATOM   1278  O   ASP D   6       2.785  96.074  19.743  1.00102.97           O
ATOM   1279  CB  ASP D   6       0.971  98.212  21.039  1.00108.00           C
ATOM   1280  CG  ASP D   6       0.074  98.200  22.274  1.00112.58           C
ATOM   1281  OD1 ASP D   6       0.237  97.269  23.096  1.00115.34           O
ATOM   1282  OD2 ASP D   6      -0.785  99.100  22.417  1.00114.32
O1-
ATOM   1283  N   GLU D   7       4.014  97.959  19.569  1.00104.18           N
ATOM   1284  CA  GLU D   7       4.799  97.481  18.439  1.00104.53           C
ATOM   1285  C   GLU D   7       5.713  96.462  19.118  1.00103.48           C
ATOM   1286  O   GLU D   7       5.970  95.376  18.591  1.00102.50           O
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ATOM   1287  CB  GLU D   7       5.617  98.638  17.849  1.00106.95           C
ATOM   1288  CG  GLU D   7       4.776  99.656  17.087  1.00110.40           C
ATOM   1289  CD  GLU D   7       4.581  99.279  15.628  1.00113.03           C
ATOM   1290  OE1 GLU D   7       5.459  99.643  14.813  1.00114.03           O
ATOM   1291  OE2 GLU D   7       3.568  98.614  15.299  1.00113.25
O1-
ATOM   1292  N   LEU D   8       6.176  96.835  20.311  1.00100.91           N
ATOM   1293  CA  LEU D   8       7.043  95.997  21.135  1.00 96.57           C
ATOM   1294  C   LEU D   8       6.300  94.770  21.645  1.00 98.57           C
ATOM   1295  O   LEU D   8       6.724  93.638  21.424  1.00100.66           O
ATOM   1296  CB  LEU D   8       7.542  96.766  22.354  1.00 89.15           C
ATOM   1297  CG  LEU D   8       8.429  97.975  22.144  1.00 82.99           C
ATOM   1298  CD1 LEU D   8       8.744  98.566  23.495  1.00 78.33           C
ATOM   1299  CD2 LEU D   8       9.689  97.577  21.412  1.00 78.68           C
ATOM   1300  N   MET D   9       5.207  94.995  22.364  1.00 98.60           N
ATOM   1301  CA  MET D   9       4.448  93.877  22.891  1.00101.80           C
ATOM   1302  C   MET D   9       4.186  92.858  21.787  1.00102.97           C
ATOM   1303  O   MET D   9       4.132  91.649  22.040  1.00102.93           O
ATOM   1304  CB  MET D   9       3.136  94.375  23.500  1.00104.99           C
ATOM   1305  CG  MET D   9       3.338  95.015  24.860  1.00106.99           C
ATOM   1306  SD  MET D   9       4.406  93.995  25.914  1.00107.55           S
ATOM   1307  CE  MET D   9       3.273  92.744  26.447  1.00108.44           C
ATOM   1308  N   ALA D  10       4.048  93.355  20.560  1.00102.71           N
ATOM   1309  CA  ALA D  10       3.801  92.510  19.397  1.00102.15           C
ATOM   1310  C   ALA D  10       5.039  91.707  18.967  1.00101.89           C
ATOM   1311  O   ALA D  10       4.906  90.592  18.466  1.00102.04           O
ATOM   1312  CB  ALA D  10       3.299  93.361  18.234  1.00 99.65           C
ATOM   1313  N   SER D  11       6.234  92.268  19.161  1.00101.68           N
ATOM   1314  CA  SER D  11       7.494  91.604  18.790  1.00100.63           C
ATOM   1315  C   SER D  11       7.695  90.245  19.463  1.00104.57           C
ATOM   1316  O   SER D  11       8.455  89.405  18.966  1.00104.79           O
ATOM   1317  CB  SER D  11       8.697  92.485  19.141  1.00 96.62           C
ATOM   1318  OG  SER D  11       8.655  93.731  18.478  1.00 92.87           O
ATOM   1319  N   LEU D  12       7.033  90.037  20.598  1.00106.92           N
ATOM   1320  CA  LEU D  12       7.154  88.781  21.337  1.00109.11           C
ATOM   1321  C   LEU D  12       5.963  87.877  21.013  1.00112.49           C
ATOM   1322  O   LEU D  12       6.125  86.686  20.730  1.00111.74           O
ATOM   1323  CB  LEU D  12       7.196  89.075  22.837  1.00108.48           C
ATOM   1324  CG  LEU D  12       8.137  90.203  23.254  1.00104.98           C
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ATOM   1325  CD1 LEU D  12       7.520  90.980  24.395  1.00100.51           C
ATOM   1326  CD2 LEU D  12       9.489  89.632  23.634  1.00104.05           C
ATOM   1327  N   SER D  13       4.603  88.435  21.039  1.00  0.00           N
ATOM   1328  CA  SER D  13       3.704  87.339  20.691  1.00  0.00           C
ATOM   1329  C   SER D  13       4.069  86.745  19.351  1.00  0.00           C
ATOM   1330  O   SER D  13       4.328  87.449  18.375  1.00  0.00           O
ATOM   1331  CB  SER D  13       2.227  87.805  20.725  1.00  0.00           C
ATOM   1332  OG  SER D  13       1.907  88.716  19.668  1.00  0.00           O
ATOM   1333  H   SER D  13       4.325  89.453  21.269  1.00  0.00           H
ATOM   1334  HA  SER D  13       3.836  86.539  21.442  1.00  0.00           H
ATOM   1335 2HB  SER D  13       1.975  88.266  21.699  1.00  0.00           H
ATOM   1336 3HB  SER D  13       1.557  86.927  20.644  1.00  0.00           H
ATOM   1337  HG  SER D  13       2.442  89.503  19.795  1.00  0.00           H
ATOM   1338  N   ASP D  14       4.115  85.283  19.207  1.00  0.00           N
ATOM   1339  CA  ASP D  14       4.490  85.019  17.821  1.00  0.00           C
ATOM   1340  C   ASP D  14       3.691  83.870  17.253  1.00  0.00           C
ATOM   1341  O   ASP D  14       3.509  82.820  17.887  1.00  0.00           O
ATOM   1342  CB  ASP D  14       6.015  84.743  17.711  1.00  0.00           C
ATOM   1343  CG  ASP D  14       6.546  84.521  16.287  1.00  0.00           C
ATOM   1344  OD1 ASP D  14       6.065  85.188  15.348  1.00  0.00           O
ATOM   1345  OD2 ASP D  14       7.415  83.643  16.104  1.00  0.00
O1-
ATOM   1346  H   ASP D  14       3.911  84.550  19.974  1.00  0.00           H
ATOM   1347  HA  ASP D  14       4.247  85.916  17.220  1.00  0.00           H
ATOM   1348 2HB  ASP D  14       6.283  83.855  18.313  1.00  0.00           H
ATOM   1349 3HB  ASP D  14       6.595  85.577  18.138  1.00  0.00           H
ATOM   1350  N   PHE D  15       3.112  84.001  15.909  1.00  0.00           N
ATOM   1351  CA  PHE D  15       2.409  82.750  15.642  1.00  0.00           C
ATOM   1352  C   PHE D  15       2.632  82.295  14.219  1.00  0.00           C
ATOM   1353  O   PHE D  15       2.554  83.092  13.243  1.00  0.00           O
ATOM   1354  CB  PHE D  15       0.879  82.935  15.876  1.00  0.00           C
ATOM   1355  CG  PHE D  15       0.453  83.400  17.278  1.00  0.00           C
ATOM   1356  CD1 PHE D  15       0.380  84.769  17.560  1.00  0.00           C
ATOM   1357  CD2 PHE D  15       0.197  82.474  18.292  1.00  0.00           C
ATOM   1358  CE1 PHE D  15       0.075  85.205  18.845  1.00  0.00           C
ATOM   1359  CE2 PHE D  15      -0.120  82.911  19.575  1.00  0.00           C
ATOM   1360  CZ  PHE D  15      -0.177  84.276  19.852  1.00  0.00           C
ATOM   1361  H   PHE D  15       3.191  84.853  15.250  1.00  0.00           H
ATOM   1362  HA  PHE D  15       2.802  81.966  16.318  1.00  0.00           H
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ATOM   1363 2HB  PHE D  15       0.354  81.987  15.648  1.00  0.00           H
ATOM   1364 3HB  PHE D  15       0.471  83.643  15.126  1.00  0.00           H
ATOM   1365 1HD  PHE D  15       0.606  85.495  16.791  1.00  0.00           H
ATOM   1366 2HD  PHE D  15       0.261  81.413  18.090  1.00  0.00           H
ATOM   1367 1HE  PHE D  15       0.052  86.263  19.060  1.00  0.00           H
ATOM   1368 2HE  PHE D  15      -0.309  82.191  20.358  1.00  0.00           H
ATOM   1369  HZ  PHE D  15      -0.409  84.617  20.849  1.00  0.00           H
ATOM   1370  N   LYS D  16       2.950  80.883  13.963  1.00  0.00           N
ATOM   1371  CA  LYS D  16       3.107  80.754  12.517  1.00  0.00           C
ATOM   1372  C   LYS D  16       2.470  79.480  12.015  1.00  0.00           C
ATOM   1373  O   LYS D  16       2.628  78.394  12.592  1.00  0.00           O
ATOM   1374  CB  LYS D  16       4.617  80.799  12.156  1.00  0.00           C
ATOM   1375  CG  LYS D  16       4.887  80.746  10.631  1.00  0.00           C
ATOM   1376  CD  LYS D  16       6.368  80.723  10.240  1.00  0.00           C
ATOM   1377  CE  LYS D  16       6.486  80.596   8.715  1.00  0.00           C
ATOM   1378  NZ  LYS D  16       7.897  80.747   8.319  1.00  0.00
N1+
ATOM   1379  H   LYS D  16       3.048  80.097  14.698  1.00  0.00           H
ATOM   1380  HA  LYS D  16       2.586  81.600  12.033  1.00  0.00           H
ATOM   1381 2HB  LYS D  16       5.147  79.966  12.662  1.00  0.00           H
ATOM   1382 3HB  LYS D  16       5.073  81.720  12.572  1.00  0.00           H
ATOM   1383 2HG  LYS D  16       4.379  81.595  10.134  1.00  0.00           H
ATOM   1384 3HG  LYS D  16       4.436  79.835  10.195  1.00  0.00           H
ATOM   1385 2HD  LYS D  16       6.874  79.869  10.735  1.00  0.00           H
ATOM   1386 3HD  LYS D  16       6.867  81.638  10.610  1.00  0.00           H
ATOM   1387 2HE  LYS D  16       5.872  81.365   8.201  1.00  0.00           H
ATOM   1388 3HE  LYS D  16       6.091  79.616   8.375  1.00  0.00           H
ATOM   1389 1HZ  LYS D  16       8.516  80.308   9.011  1.00  0.00           H
ATOM   1390 2HZ  LYS D  16       8.087  80.277   7.428  1.00  0.00           H
ATOM   1391 3HZ  LYS D  16       8.067  81.740   8.246  1.00  0.00           H
ATOM   1392  N   PHE D  17       1.636  79.529  10.805  1.00  0.00           N
ATOM   1393  CA  PHE D  17       1.168  78.166  10.575  1.00  0.00           C
ATOM   1394  C   PHE D  17       1.211  77.819   9.106  1.00  0.00           C
ATOM   1395  O   PHE D  17       0.791  78.614   8.219  1.00  0.00           O
ATOM   1396  CB  PHE D  17      -0.297  78.010  11.086  1.00  0.00           C
ATOM   1397  CG  PHE D  17      -0.541  78.323  12.571  1.00  0.00           C
ATOM   1398  CD1 PHE D  17      -0.839  79.634  12.960  1.00  0.00           C
ATOM   1399  CD2 PHE D  17      -0.408  77.329  13.543  1.00  0.00           C
ATOM   1400  CE1 PHE D  17      -0.983  79.950  14.307  1.00  0.00           C
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ATOM   1401  CE2 PHE D  17      -0.563  77.644  14.891  1.00  0.00           C
ATOM   1402  CZ  PHE D  17      -0.847  78.954  15.272  1.00  0.00           C
ATOM   1403  H   PHE D  17       1.414  80.400  10.207  1.00  0.00           H
ATOM   1404  HA  PHE D  17       1.832  77.463  11.113  1.00  0.00           H
ATOM   1405 2HB  PHE D  17      -0.649  76.979  10.884  1.00  0.00           H
ATOM   1406 3HB  PHE D  17      -0.974  78.638  10.472  1.00  0.00           H
ATOM   1407 1HD  PHE D  17      -0.914  80.418  12.219  1.00  0.00           H
ATOM   1408 2HD  PHE D  17      -0.166  76.315  13.256  1.00  0.00           H
ATOM   1409 1HE  PHE D  17      -1.182  80.970  14.599  1.00  0.00           H
ATOM   1410 2HE  PHE D  17      -0.451  76.874  15.640  1.00  0.00           H
ATOM   1411  HZ  PHE D  17      -0.954  79.203  16.317  1.00  0.00           H
ATOM   1412  N   MET D  18       1.758  76.518   8.696  1.00  0.00           N
ATOM   1413  CA  MET D  18       1.666  76.475   7.239  1.00  0.00           C
ATOM   1414  C   MET D  18       1.221  75.114   6.763  1.00  0.00           C
ATOM   1415  O   MET D  18       0.979  74.189   7.554  1.00  0.00           O
ATOM   1416  CB  MET D  18       3.035  76.861   6.614  1.00  0.00           C
ATOM   1417  CG  MET D  18       3.535  78.291   6.914  1.00  0.00           C
ATOM   1418  SD  MET D  18       4.966  78.665   5.889  1.00  0.00           S
ATOM   1419  CE  MET D  18       5.514  80.156   6.732  1.00  0.00           C
ATOM   1420  H   MET D  18       2.149  75.747   9.343  1.00  0.00           H
ATOM   1421  HA  MET D  18       0.898  77.201   6.913  1.00  0.00           H
ATOM   1422 2HB  MET D  18       2.980  76.748   5.514  1.00  0.00           H
ATOM   1423 3HB  MET D  18       3.813  76.139   6.934  1.00  0.00           H
ATOM   1424 2HG  MET D  18       3.815  78.379   7.981  1.00  0.00           H
ATOM   1425 3HG  MET D  18       2.747  79.044   6.729  1.00  0.00           H
ATOM   1426 1HE  MET D  18       4.706  80.907   6.774  1.00  0.00           H
ATOM   1427 2HE  MET D  18       5.826  79.921   7.765  1.00  0.00           H
ATOM   1428 3HE  MET D  18       6.376  80.602   6.206  1.00  0.00           H
TER    1429      MET D  18
HETATM 1430  O   HOH D  37       2.384 105.217  19.682  1.00 71.42           O
HETATM 1431  O   HOH D 111      10.178  87.969  17.399  1.00 73.03           O
ATOM   1432  N   SER F  -3       3.544  97.175  60.553  1.00  0.00           N
ATOM   1433  CA  SER F  -3       3.529  96.933  59.114  1.00  0.00           C
ATOM   1434  C   SER F  -3       4.914  97.074  58.527  1.00  0.00           C
ATOM   1435  O   SER F  -3       5.655  98.011  58.824  1.00  0.00           O
ATOM   1436  CB  SER F  -3       2.513  97.867  58.409  1.00  0.00           C
ATOM   1437  OG  SER F  -3       2.923  99.239  58.413  1.00  0.00           O
ATOM   1438  H   SER F  -3       4.452  97.419  61.084  1.00  0.00           H
ATOM   1439  HA  SER F  -3       3.215  95.886  58.947  1.00  0.00           H
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ATOM   1440 2HB  SER F  -3       1.508  97.781  58.863  1.00  0.00           H
ATOM   1441 3HB  SER F  -3       2.380  97.547  57.357  1.00  0.00           H
ATOM   1442  HG  SER F  -3       2.963  99.524  59.329  1.00  0.00           H
ATOM   1443  N   ALA F  -2       5.331  96.187  57.689  1.00  0.00           N
ATOM   1444  CA  ALA F  -2       6.677  96.376  57.155  1.00  0.00           C
ATOM   1445  C   ALA F  -2       6.723  96.055  55.680  1.00  0.00           C
ATOM   1446  O   ALA F  -2       6.554  94.907  55.252  1.00  0.00           O
ATOM   1447  CB  ALA F  -2       7.635  95.503  57.984  1.00  0.00           C
ATOM   1448  H   ALA F  -2       4.717  95.348  57.397  1.00  0.00           H
ATOM   1449  HA  ALA F  -2       6.957  97.440  57.269  1.00  0.00           H
ATOM   1450 1HB  ALA F  -2       7.615  95.777  59.057  1.00  0.00           H
ATOM   1451 2HB  ALA F  -2       7.379  94.427  57.922  1.00  0.00           H
ATOM   1452 3HB  ALA F  -2       8.683  95.608  57.649  1.00  0.00           H
ATOM   1453  N   SER F  -1       6.977  97.142  54.723  1.00  0.00           N
ATOM   1454  CA  SER F  -1       6.963  96.531  53.397  1.00  0.00           C
ATOM   1455  C   SER F  -1       8.295  96.705  52.707  1.00  0.00           C
ATOM   1456  O   SER F  -1       8.708  97.810  52.355  1.00  0.00           O
ATOM   1457  CB  SER F  -1       5.800  97.095  52.542  1.00  0.00           C
ATOM   1458  OG  SER F  -1       5.997  98.463  52.168  1.00  0.00           O
ATOM   1459  H   SER F  -1       7.141  98.184  54.954  1.00  0.00           H
ATOM   1460  HA  SER F  -1       6.808  95.443  53.524  1.00  0.00           H
ATOM   1461 2HB  SER F  -1       4.831  96.991  53.066  1.00  0.00           H
ATOM   1462 3HB  SER F  -1       5.691  96.493  51.619  1.00  0.00           H
ATOM   1463  HG  SER F  -1       6.017  98.982  52.976  1.00  0.00           H
ATOM   1464  N   SER F   0       9.022  95.664  52.479  1.00  0.00           N
ATOM   1465  CA  SER F   0      10.311  95.829  51.812  1.00  0.00           C
ATOM   1466  C   SER F   0      10.344  95.071  50.505  1.00  0.00           C
ATOM   1467  O   SER F   0       9.925  93.918  50.409  1.00  0.00           O
ATOM   1468  CB  SER F   0      11.473  95.406  52.745  1.00  0.00           C
ATOM   1469  OG  SER F   0      11.510  93.995  52.983  1.00  0.00           O
ATOM   1470  H   SER F   0       8.683  94.683  52.777  1.00  0.00           H
ATOM   1471  HA  SER F   0      10.432  96.899  51.565  1.00  0.00           H
ATOM   1472 2HB  SER F   0      11.425  95.942  53.712  1.00  0.00           H
ATOM   1473 3HB  SER F   0      12.439  95.710  52.298  1.00  0.00           H
ATOM   1474  HG  SER F   0      10.698  93.758  53.438  1.00  0.00           H
ATOM   1475  N   ALA F   1      10.826  95.651  49.458  1.00  0.00           N
ATOM   1476  CA  ALA F   1      10.832  94.870  48.224  1.00  0.00           C
ATOM   1477  C   ALA F   1      12.118  95.077  47.461  1.00  0.00           C
ATOM   1478  O   ALA F   1      12.764  94.131  46.995  1.00  0.00           O
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ATOM   1479  CB  ALA F   1       9.587  95.269  47.414  1.00  0.00           C
ATOM   1480  H   ALA F   1      11.206  96.662  49.493  1.00  0.00           H
ATOM   1481  HA  ALA F   1      10.774  93.797  48.485  1.00  0.00           H
ATOM   1482 1HB  ALA F   1       8.653  95.075  47.975  1.00  0.00           H
ATOM   1483 2HB  ALA F   1       9.588  96.344  47.150  1.00  0.00           H
ATOM   1484 3HB  ALA F   1       9.512  94.702  46.468  1.00  0.00           H
ATOM   1485  N   THR F   2      12.618  96.446  47.265  1.00167.72           N
ATOM   1486  CA  THR F   2      13.892  96.405  46.489  1.00168.68           C
ATOM   1487  C   THR F   2      14.921  95.534  47.201  1.00168.68           C
ATOM   1488  O   THR F   2      15.977  95.221  46.647  1.00168.77           O
ATOM   1489  CB  THR F   2      14.477  97.825  46.307  1.00169.03           C
ATOM   1490  CG2 THR F   2      15.821  97.770  45.586  1.00169.26           C
ATOM   1491  OG1 THR F   2      13.563  98.626  45.545  1.00170.92           O
ATOM   1492  N   ARG F   3      14.607  95.142  48.431  1.00168.25           N
ATOM   1493  CA  ARG F   3      15.506  94.304  49.213  1.00167.59           C
ATOM   1494  C   ARG F   3      15.429  92.866  48.694  1.00168.72           C
ATOM   1495  O   ARG F   3      16.417  92.131  48.745  1.00169.37           O
ATOM   1496  CB  ARG F   3      15.122  94.374  50.695  1.00165.45           C
ATOM   1497  CG  ARG F   3      16.317  94.416  51.642  1.00163.06           C
ATOM   1498  CD  ARG F   3      15.889  94.705  53.078  1.00161.21           C
ATOM   1499  NE  ARG F   3      15.607  96.119  53.329  1.00159.22           N
ATOM   1500  CZ  ARG F   3      15.015  96.572  54.430  1.00158.39           C
ATOM   1501  NH1 ARG F   3      14.639  95.720  55.375  1.00157.72
N1+
ATOM   1502  NH2 ARG F   3      14.812  97.874  54.598  1.00157.85           N
ATOM   1503  N   GLU F   4      14.255  92.484  48.184  1.00169.29           N
ATOM   1504  CA  GLU F   4      14.025  91.146  47.628  1.00168.31           C
ATOM   1505  C   GLU F   4      14.487  91.112  46.170  1.00167.94           C
ATOM   1506  O   GLU F   4      14.764  90.045  45.609  1.00166.98           O
ATOM   1507  CB  GLU F   4      12.540  90.787  47.687  1.00167.80           C
ATOM   1508  CG  GLU F   4      11.896  90.899  49.060  1.00167.27           C
ATOM   1509  CD  GLU F   4      10.579  90.140  49.139  1.00168.28           C
ATOM   1510  OE1 GLU F   4       9.703  90.366  48.276  1.00167.92           O
ATOM   1511  OE2 GLU F   4      10.420  89.316  50.065  1.00168.81
O1-
ATOM   1512  N   LEU F   5      14.553  92.296  45.567  1.00167.58           N
ATOM   1513  CA  LEU F   5      15.002  92.453  44.189  1.00167.99           C
ATOM   1514  C   LEU F   5      16.537  92.441  44.166  1.00169.16           C
ATOM   1515  O   LEU F   5      17.157  92.024  43.182  1.00168.77           O
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ATOM   1516  CB  LEU F   5      14.478  93.774  43.624  1.00166.25           C
ATOM   1517  CG  LEU F   5      14.988  94.231  42.257  1.00165.05           C
ATOM   1518  CD1 LEU F   5      14.468  93.324  41.150  1.00163.55           C
ATOM   1519  CD2 LEU F   5      14.538  95.656  42.032  1.00164.01           C
ATOM   1520  N   ASP F   6      17.140  92.897  45.263  1.00169.94           N
ATOM   1521  CA  ASP F   6      18.595  92.933  45.391  1.00169.64           C
ATOM   1522  C   ASP F   6      19.138  91.563  45.758  1.00169.28           C
ATOM   1523  O   ASP F   6      20.317  91.278  45.546  1.00168.18           O
ATOM   1524  CB  ASP F   6      19.023  93.965  46.434  1.00170.12           C
ATOM   1525  CG  ASP F   6      18.893  95.385  45.925  1.00172.08           C
ATOM   1526  OD1 ASP F   6      19.227  95.615  44.741  1.00172.61           O
ATOM   1527  OD2 ASP F   6      18.470  96.269  46.701  1.00173.49
O1-
ATOM   1528  N   GLU F   7      18.272  90.725  46.321  1.00169.63           N
ATOM   1529  CA  GLU F   7      18.642  89.358  46.664  1.00169.36           C
ATOM   1530  C   GLU F   7      18.916  88.778  45.282  1.00169.37           C
ATOM   1531  O   GLU F   7      19.858  88.009  45.071  1.00169.25           O
ATOM   1532  CB  GLU F   7      17.453  88.619  47.297  1.00169.43           C
ATOM   1533  CG  GLU F   7      16.960  89.198  48.617  1.00168.79           C
ATOM   1534  CD  GLU F   7      17.596  88.538  49.825  1.00168.60           C
ATOM   1535  OE1 GLU F   7      17.092  87.480  50.260  1.00167.14           O
ATOM   1536  OE2 GLU F   7      18.606  89.071  50.333  1.00168.56
O1-
ATOM   1537  N   LEU F   8      18.069  89.199  44.345  1.00168.60           N
ATOM   1538  CA  LEU F   8      18.125  88.783  42.951  1.00167.55           C
ATOM   1539  C   LEU F   8      19.321  89.384  42.207  1.00168.46           C
ATOM   1540  O   LEU F   8      20.059  88.662  41.530  1.00168.63           O
ATOM   1541  CB  LEU F   8      16.817  89.177  42.252  1.00164.51           C
ATOM   1542  CG  LEU F   8      15.527  88.563  42.814  1.00161.82           C
ATOM   1543  CD1 LEU F   8      14.310  89.243  42.215  1.00160.14           C
ATOM   1544  CD2 LEU F   8      15.500  87.079  42.514  1.00161.14           C
ATOM   1545  N   MET F   9      19.517  90.696  42.341  1.00169.27           N
ATOM   1546  CA  MET F   9      20.623  91.381  41.671  1.00170.34           C
ATOM   1547  C   MET F   9      21.990  90.920  42.196  1.00170.50           C
ATOM   1548  O   MET F   9      23.015  91.080  41.523  1.00170.08           O
ATOM   1549  CB  MET F   9      20.474  92.903  41.821  1.00171.17           C
ATOM   1550  CG  MET F   9      19.210  93.489  41.164  1.00172.23           C
ATOM   1551  SD  MET F   9      18.947  93.057  39.408  1.00173.00           S
ATOM   1552  CE  MET F   9      20.201  94.088  38.567  1.00172.02           C
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ATOM   1553  N   ALA F  10      21.988  90.333  43.391  1.00170.19           N
ATOM   1554  CA  ALA F  10      23.204  89.820  44.021  1.00169.09           C
ATOM   1555  C   ALA F  10      23.472  88.382  43.568  1.00168.90           C
ATOM   1556  O   ALA F  10      24.601  87.896  43.636  1.00167.06           O
ATOM   1557  CB  ALA F  10      23.064  89.874  45.540  1.00167.81           C
ATOM   1558  N   SER F  11      22.421  87.707  43.109  1.00169.78           N
ATOM   1559  CA  SER F  11      22.528  86.331  42.633  1.00169.93           C
ATOM   1560  C   SER F  11      23.397  86.282  41.387  1.00171.22           C
ATOM   1561  O   SER F  11      24.118  85.313  41.152  1.00170.34           O
ATOM   1562  CB  SER F  11      21.141  85.771  42.307  1.00168.77           C
ATOM   1563  OG  SER F  11      20.351  85.639  43.473  1.00167.98           O
ATOM   1564  N   LEU F  12      23.313  87.341  40.589  1.00173.79           N
ATOM   1565  CA  LEU F  12      24.082  87.455  39.358  1.00176.17           C
ATOM   1566  C   LEU F  12      25.519  87.870  39.666  1.00178.24           C
ATOM   1567  O   LEU F  12      26.470  87.285  39.146  1.00179.14           O
ATOM   1568  CB  LEU F  12      23.418  88.481  38.435  1.00175.22           C
ATOM   1569  CG  LEU F  12      21.974  88.127  38.071  1.00174.35           C
ATOM   1570  CD1 LEU F  12      21.284  89.305  37.400  1.00173.85           C
ATOM   1571  CD2 LEU F  12      21.982  86.906  37.169  1.00173.97           C
ATOM   1572  N   SER F  13      25.770  88.982  40.594  1.00  0.00           N
ATOM   1573  CA  SER F  13      27.221  89.127  40.675  1.00  0.00           C
ATOM   1574  C   SER F  13      27.870  87.837  41.117  1.00  0.00           C
ATOM   1575  O   SER F  13      27.425  87.171  42.052  1.00  0.00           O
ATOM   1576  CB  SER F  13      27.606  90.306  41.604  1.00  0.00           C
ATOM   1577  OG  SER F  13      27.318  90.046  42.982  1.00  0.00           O
ATOM   1578  H   SER F  13      25.030  89.573  41.112  1.00  0.00           H
ATOM   1579  HA  SER F  13      27.599  89.344  39.659  1.00  0.00           H
ATOM   1580 2HB  SER F  13      27.104  91.242  41.292  1.00  0.00           H
ATOM   1581 3HB  SER F  13      28.689  90.518  41.507  1.00  0.00           H
ATOM   1582  HG  SER F  13      26.368  89.937  43.062  1.00  0.00           H
ATOM   1583  N   ASP F  14      29.068  87.362  40.410  1.00  0.00           N
ATOM   1584  CA  ASP F  14      29.457  86.112  41.056  1.00  0.00           C
ATOM   1585  C   ASP F  14      30.955  86.027  41.215  1.00  0.00           C
ATOM   1586  O   ASP F  14      31.732  86.330  40.295  1.00  0.00           O
ATOM   1587  CB  ASP F  14      28.913  84.893  40.259  1.00  0.00           C
ATOM   1588  CG  ASP F  14      29.196  83.518  40.881  1.00  0.00           C
ATOM   1589  OD1 ASP F  14      29.159  83.392  42.122  1.00  0.00           O
ATOM   1590  OD2 ASP F  14      29.502  82.572  40.124  1.00  0.00
O1-
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ATOM   1591  H   ASP F  14      29.562  87.843  39.579  1.00  0.00           H
ATOM   1592  HA  ASP F  14      29.018  86.096  42.072  1.00  0.00           H
ATOM   1593 2HB  ASP F  14      29.331  84.893  39.236  1.00  0.00           H
ATOM   1594 3HB  ASP F  14      27.820  84.964  40.135  1.00  0.00           H
ATOM   1595  N   PHE F  15      31.512  85.573  42.497  1.00  0.00           N
ATOM   1596  CA  PHE F  15      32.964  85.597  42.345  1.00  0.00           C
ATOM   1597  C   PHE F  15      33.596  84.385  42.986  1.00  0.00           C
ATOM   1598  O   PHE F  15      33.578  84.204  44.236  1.00  0.00           O
ATOM   1599  CB  PHE F  15      33.550  86.880  43.009  1.00  0.00           C
ATOM   1600  CG  PHE F  15      33.022  88.225  42.485  1.00  0.00           C
ATOM   1601  CD1 PHE F  15      31.875  88.788  43.058  1.00  0.00           C
ATOM   1602  CD2 PHE F  15      33.634  88.861  41.403  1.00  0.00           C
ATOM   1603  CE1 PHE F  15      31.338  89.962  42.542  1.00  0.00           C
ATOM   1604  CE2 PHE F  15      33.102  90.043  40.894  1.00  0.00           C
ATOM   1605  CZ  PHE F  15      31.953  90.591  41.462  1.00  0.00           C
ATOM   1606  H   PHE F  15      30.958  85.281  43.376  1.00  0.00           H
ATOM   1607  HA  PHE F  15      33.212  85.583  41.267  1.00  0.00           H
ATOM   1608 2HB  PHE F  15      34.653  86.875  42.908  1.00  0.00           H
ATOM   1609 3HB  PHE F  15      33.391  86.837  44.106  1.00  0.00           H
ATOM   1610 1HD  PHE F  15      31.375  88.288  43.877  1.00  0.00           H
ATOM   1611 2HD  PHE F  15      34.513  88.430  40.943  1.00  0.00           H
ATOM   1612 1HE  PHE F  15      30.436  90.372  42.972  1.00  0.00           H
ATOM   1613 2HE  PHE F  15      33.574  90.527  40.052  1.00  0.00           H
ATOM   1614  HZ  PHE F  15      31.531  91.500  41.060  1.00  0.00           H
ATOM   1615  N   LYS F  16      34.251  83.385  42.130  1.00  0.00           N
ATOM   1616  CA  LYS F  16      34.758  82.349  43.025  1.00  0.00           C
ATOM   1617  C   LYS F  16      36.261  82.233  42.923  1.00  0.00           C
ATOM   1618  O   LYS F  16      36.820  81.827  41.894  1.00  0.00           O
ATOM   1619  CB  LYS F  16      34.073  80.996  42.689  1.00  0.00           C
ATOM   1620  CG  LYS F  16      34.489  79.843  43.636  1.00  0.00           C
ATOM   1621  CD  LYS F  16      33.882  78.478  43.295  1.00  0.00           C
ATOM   1622  CE  LYS F  16      34.433  77.424  44.263  1.00  0.00           C
ATOM   1623  NZ  LYS F  16      33.727  76.148  44.052  1.00  0.00
N1+
ATOM   1624  H   LYS F  16      34.340  83.413  41.054  1.00  0.00           H
ATOM   1625  HA  LYS F  16      34.517  82.636  44.065  1.00  0.00           H
ATOM   1626 2HB  LYS F  16      34.292  80.718  41.638  1.00  0.00           H
ATOM   1627 3HB  LYS F  16      32.972  81.116  42.727  1.00  0.00           H
ATOM   1628 2HG  LYS F  16      34.243  80.114  44.681  1.00  0.00           H
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ATOM   1629 3HG  LYS F  16      35.586  79.710  43.617  1.00  0.00           H
ATOM   1630 2HD  LYS F  16      34.134  78.207  42.249  1.00  0.00           H
ATOM   1631 3HD  LYS F  16      32.778  78.536  43.344  1.00  0.00           H
ATOM   1632 2HE  LYS F  16      34.311  77.746  45.318  1.00  0.00           H
ATOM   1633 3HE  LYS F  16      35.526  77.291  44.112  1.00  0.00           H
ATOM   1634 1HZ  LYS F  16      33.526  76.006  43.055  1.00  0.00           H
ATOM   1635 2HZ  LYS F  16      34.301  75.351  44.344  1.00  0.00           H
ATOM   1636 3HZ  LYS F  16      32.878  76.199  44.597  1.00  0.00           H
ATOM   1637  N   PHE F  17      37.085  82.614  44.079  1.00  0.00           N
ATOM   1638  CA  PHE F  17      38.473  82.396  43.682  1.00  0.00           C
ATOM   1639  C   PHE F  17      39.137  81.373  44.573  1.00  0.00           C
ATOM   1640  O   PHE F  17      39.363  81.598  45.795  1.00  0.00           O
ATOM   1641  CB  PHE F  17      39.270  83.733  43.770  1.00  0.00           C
ATOM   1642  CG  PHE F  17      38.740  84.903  42.926  1.00  0.00           C
ATOM   1643  CD1 PHE F  17      37.777  85.764  43.465  1.00  0.00           C
ATOM   1644  CD2 PHE F  17      39.160  85.080  41.606  1.00  0.00           C
ATOM   1645  CE1 PHE F  17      37.228  86.778  42.687  1.00  0.00           C
ATOM   1646  CE2 PHE F  17      38.618  86.103  40.831  1.00  0.00           C
ATOM   1647  CZ  PHE F  17      37.651  86.948  41.371  1.00  0.00           C
ATOM   1648  H   PHE F  17      36.734  82.981  45.032  1.00  0.00           H
ATOM   1649  HA  PHE F  17      38.493  82.012  42.645  1.00  0.00           H
ATOM   1650 2HB  PHE F  17      40.326  83.551  43.489  1.00  0.00           H
ATOM   1651 3HB  PHE F  17      39.337  84.058  44.829  1.00  0.00           H
ATOM   1652 1HD  PHE F  17      37.422  85.617  44.476  1.00  0.00           H
ATOM   1653 2HD  PHE F  17      39.894  84.415  41.173  1.00  0.00           H
ATOM   1654 1HE  PHE F  17      36.464  87.417  43.103  1.00  0.00           H
ATOM   1655 2HE  PHE F  17      38.941  86.232  39.808  1.00  0.00           H
ATOM   1656  HZ  PHE F  17      37.219  87.733  40.767  1.00  0.00           H
ATOM   1657  N   MET F  18      39.532  80.078  44.000  1.00  0.00           N
ATOM   1658  CA  MET F  18      40.139  79.317  45.089  1.00  0.00           C
ATOM   1659  C   MET F  18      41.576  78.977  44.777  1.00  0.00           C
ATOM   1660  O   MET F  18      42.118  79.326  43.717  1.00  0.00           O
ATOM   1661  CB  MET F  18      39.310  78.031  45.358  1.00  0.00           C
ATOM   1662  CG  MET F  18      37.854  78.251  45.823  1.00  0.00           C
ATOM   1663  SD  MET F  18      37.143  76.689  46.363  1.00  0.00           S
ATOM   1664  CE  MET F  18      35.420  77.195  46.445  1.00  0.00           C
ATOM   1665  H   MET F  18      39.401  79.755  42.978  1.00  0.00           H
ATOM   1666  HA  MET F  18      40.144  79.946  45.999  1.00  0.00           H
ATOM   1667 2HB  MET F  18      39.820  77.421  46.127  1.00  0.00           H
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ATOM   1668 3HB  MET F  18      39.300  77.393  44.451  1.00  0.00           H
ATOM   1669 2HG  MET F  18      37.249  78.662  44.993  1.00  0.00           H
ATOM   1670 3HG  MET F  18      37.798  78.983  46.650  1.00  0.00           H
ATOM   1671 1HE  MET F  18      35.295  78.070  47.109  1.00  0.00           H
ATOM   1672 2HE  MET F  18      35.050  77.465  45.440  1.00  0.00           H
ATOM   1673 3HE  MET F  18      34.793  76.373  46.833  1.00  0.00           H
TER    1674      MET F  18
HETATM 1675  O   HOH F 105      11.710  93.548  46.450  1.00 87.72           O
END
```

Appendix B. Mdp Simulation Files

1. Mdp file used for equilibrium simulations where P1/P2 unconstrained:

```
title        = MD production
; this is loosely based off of the VT pulling tutorial; heavily modified
; Run parameters
integrator   = md
dt           = 0.002
tinit        = 0
nsteps       = 5000000    ; 10 ns
; Output parameters
nstxout             = 1000       ; every 2 ps
nstvout             = 1000
nstfout             = 5000
nstxtcout    = 5000       ; every 1 ps
nstenergy    = 1000
; Bond parameters
constraint_algorithm       = lincs
constraints         = hbonds
lincs_iter      = 1              ; accuracy of LINCS
lincs_order     = 4              ; also related to accuracy
; Single-range cutoff scheme
nstlist             = 5
ns_type             = grid
rlist        = 1.4
rcoulomb     = 1.4
rvdw         = 1.4
; PME electrostatics parameters
coulombtype  = PME
fourierspacing  = 0.16
pme_order    = 4
ewald_rtol   = 1e-5
optimize_fft = yes
; Berendsen temperature coupling is on in two groups
Tcoupl       = Nose-Hoover
tc_grps             = Protein Non-Protein
tau_t        = 0.2 0.2
ref_t        = 310 310
; Pressure coupling is on
Pcoupl       = Parrinello-Rahman
pcoupltype   = isotropic
tau_p        = 1.0
compressibility     = 4.5e-5
ref_p        = 1.0
; Generate velocities is off
gen_vel             = no
; Periodic boundary conditions are on in all directions
pbc          = xyz
; Long-range dispersion correction
DispCorr     = EnerPres
; COM motion removal
```

```
; These options remove COM motion of the system
nstcomm         = 1
comm-mode       = Linear
comm-grps       = System
```

2. Mdp file used for equilibrium simulations where P1/P2 constrained:

```
title        = MD production
; this is loosely based off of the VT pulling tutorial; heavily modified
; Run parameters
integrator    = md
freezegrps = freeze
freezedim = Y Y Y
dt           = 0.002
tinit        = 0
nsteps       = 2500000    ; 5 ns
; Output parameters
nstxout             = 1000       ; every 2 ps
nstvout             = 1000
nstfout             = 5000
nstxtcout    = 5000       ; every 1 ps
nstenergy    = 1000
; Bond parameters
constraint_algorithm       = lincs
constraints         = hbonds
lincs_iter      = 1              ; accuracy of LINCS
lincs_order     = 4              ; also related to accuracy
; Single-range cutoff scheme
nstlist             = 5
ns_type             = grid
rlist        = 1.4
rcoulomb     = 1.4
rvdw         = 1.4
; PME electrostatics parameters
coulombtype  = PME
fourierspacing  = 0.16
pme_order    = 4
ewald_rtol   = 1e-5
optimize_fft = yes
; Berendsen temperature coupling is on in two groups
Tcoupl       = Nose-Hoover
tc_grps             = Protein Non-Protein
tau_t        = 0.2 0.2
ref_t        = 310 310
; Pressure coupling is on
Pcoupl       = Parrinello-Rahman
pcoupltype   = isotropic
tau_p        = 1.0
compressibility     = 4.5e-5
ref_p        = 1.0
; Generate velocities is ON
gen_vel         = yes
gen_temp        = 310
gen_seed        = -1
```

```
; Periodic boundary conditions are on in all directions
pbc          = xyz
; Long-range dispersion correction
DispCorr     = EnerPres
; COM motion removal
; These options remove COM motion of the system
nstcomm          = 1
comm-mode        = Linear
comm-grps        = System
```

3. Mdp file used for axial load scenario:

```
title        = smd_100 ; 100 pN
; this is loosely based off of the VT pulling tutorial; heavily modified
; Run parameters
integrator   = md
freezegrps = freeze
freezedim = Y Y Y
dt           = 0.002
tinit        = 0
nsteps       = 2500000    ; 5 ns
; Output parameters
nstxout             = 1000       ; every  2 ps
nstvout             = 1000
nstfout             = 5000
nstxtcout    = 5000       ; every ps
nstenergy    = 1000
; Bond parameters
constraint_algorithm       = lincs
constraints         = hbonds
lincs_iter      = 1              ; accuracy of LINCS
lincs_order     = 4              ; also related to accuracy
; Single-range cutoff scheme
nstlist             = 5
ns_type             = grid
rlist        = 1.4
rcoulomb     = 1.4
rvdw         = 1.4
; PME electrostatics parameters
coulombtype  = PME
fourierspacing  = 0.16
pme_order    = 4
ewald_rtol   = 1e-5
optimize_fft  = yes
; Berendsen temperature coupling is on in two groups
Tcoupl       = Nose-Hoover
tc_grps             = Protein Non-Protein
tau_t        = 0.2 0.2
ref_t        = 310 310
; Pressure coupling is on
Pcoupl       = Parrinello-Rahman
pcoupltype   = isotropic
tau_p        = 1.0
compressibility     = 4.5e-5
ref_p        = 1.0
```

```
; Generate velocities is ON
gen_vel         = yes
gen_temp        = 310
gen_seed        = -1
; Periodic boundary conditions are on in all directions
pbc          = xyz
; Long-range dispersion correction
DispCorr     = EnerPres
; COM motion removal
; These options remove comm motion of the constraint / freeze group
nstcomm         = 1
comm_mode       = Linear
comm_grps       = System
; pull parameters
pull            = constant_force
pull_geometry   = direction
pull_nstxout    = 500 ; will print the c.o.m. coordinates
pull_nstfout    = 500 ; forces on group
pull_ngroups    = 1
pull_group0     = Protein ;
pull_group1     = group_B ;
pull_pbcatom1   = 5 ; the CA of the 10th residue
pull_vec1       = 0.75 -1.19 -0.55 ; direction of pull, will be normalized
pull_k1         = 60.24 ; pull_k1*1.66 = 100 pN;  units: [kJ / (mol * nm^2)]
```

4. Mdp file used for perpendicular load scenario:

```
title        = smd_100 ; 100 pN
; this is loosely based off of the VT pulling tutorial; heavily modified
; Run parameters
integrator   = md
freezegrps = freeze
freezedim = Y Y Y
dt           = 0.002
tinit        = 0
nsteps       = 2500000    ; 5 ns
; Output parameters
nstxout             = 1000       ; every  2 ps
nstvout             = 1000
nstfout             = 5000
nstxtcout    = 5000       ; every ps
nstenergy    = 1000
; Bond parameters
constraint_algorithm       = lincs
constraints         = hbonds
lincs_iter      = 1              ; accuracy of LINCS
lincs_order     = 4              ; also related to accuracy
; Single-range cutoff scheme
nstlist             = 5
ns_type             = grid
rlist        = 1.4
rcoulomb     = 1.4
rvdw         = 1.4
; PME electrostatics parameters
```

```
coulombtype   = PME
fourierspacing  = 0.16
pme_order     = 4
ewald_rtol    = 1e-5
optimize_fft  = yes
; Berendsen temperature coupling is on in two groups
Tcoupl        = Nose-Hoover
tc_grps             = Protein Non-Protein
tau_t         = 0.2 0.2
ref_t         = 310 310
; Pressure coupling is on
Pcoupl        = Parrinello-Rahman
pcoupltype    = isotropic
tau_p         = 1.0
compressibility     = 4.5e-5
ref_p         = 1.0
; Generate velocities is ON
gen_vel          = yes
gen_temp         = 310
gen_seed         = -1

; Periodic boundary conditions are on in all directions
pbc           = xyz
; Long-range dispersion correction
DispCorr      = EnerPres
; COM motion removal
; These options remove comm motion of the constraint / freeze group
nstcomm          = 1
comm_mode        = Linear
comm_grps        = System
; pull parameters
pull             = constant_force
pull_geometry    = direction
pull_nstxout     = 500 ; will print the c.o.m. coordinates
pull_nstfout     = 500 ; forces on group
pull_ngroups     = 1
pull_group0      = Protein ;
pull_group1      = group_B ;
pull_pbcatom1    = 5 ; the CA of the 10th residue
pull_vec1        = 0.07 -0.31 0.92 ; direction of pull, will be normalized
pull_k1          = 60.24 ; pull_k1*1.66 = 100 pN;  units: [kJ / (mol * nm^2)]
```

Appendix C. MATLAB Codes

1. H1 Position MATLAB Code:

```
clear all;
close all;

% file name;
filename='xxxxxxxx';


% Constants;
% ---------
Average=10;  % How many points you want to average (moving average)
N=2;         % How many distance you want to calculate
R=36;        % The row that you want readfile to start with
C=0;         % The column that you want readfile to start with



% number of columns to compare
numcomp=1;

% For energy plots:
%-----------------
Xmin= 0;
Xmax= 1.5;
Ymin= 0;
Ymax= 1.5;
stepsize=0.01;


% load data for 1st file:
dat=dlmread([filename '.csv'], '\t',R,C);

% what the size of my matrix
sz=size(dat);
sz(1);
moving=sz(1)-Average+1;


% The calculation of the distances:
% ---------------------------------
for i=1:sz(1);

    for L=1:1:N;
        p=2;
        x=dat(i,p)-0.5*(dat(i,p+6)+dat(i,p+12));
        y=dat(i,p+1)-0.5*(dat(i,p+7)+dat(i,p+13));
        z=dat(i,p+2)-0.5*(dat(i,p+8)+dat(i,p+14));
        Dtop(i,L)=sqrt(x^2+y^2+z^2);
```

```
        p=p+3;
        x=dat(i,p)-0.5*(dat(i,p+6)+dat(i,p+12));
        y=dat(i,p+1)-0.5*(dat(i,p+7)+dat(i,p+13));
        z=dat(i,p+2)-0.5*(dat(i,p+8)+dat(i,p+14));
        Dbottom(i,L)=sqrt(x^2+y^2+z^2);

    end
end

D1ave=zeros(moving,1);
D2ave=zeros(moving,1);

if Average>1;
       for i=1:moving;
                for c=0:1:Average-1;
                    D1ave(i)=D1ave(i)+Dtop(i+c);
                    D2ave(i)=D2ave(i)+Dbottom(i+c);
                end
            D1ave(i)=D1ave(i)/Average;
            D2ave(i)=D2ave(i)/Average;

       end
end


divsx=(-Xmin+Xmax)/stepsize;
divsy=(-Ymin+Ymax)/stepsize;

for i=1:divsx
    for j=1:divsy
        hist(i,j)=0;
    end
end

tot=0;

compmat=[1 2];

    % loop through images (this part of script was taken from Steven script)
    for n=1:moving

    % evaluate dat1; data in column specified by first entry of 'compmat'
        D1ave(n)
                x=round((D1ave(n)-Xmin)/stepsize);
        D2ave(n)
    % evaluate dat2; data in column specified by second entry of 'compmat'
                y=round((D2ave(n)-Ymin)/stepsize);

    % update histogram if within limits

        if ((x>0)&&(x<divsx))&&((y>0)&&(y<divsy))
                    hist(x,y)=hist(x,y)+1;
                    tot=tot+1;
        end

    end


% end loop over distances
```

```
pdf2d=hist/(tot-1);

% convert pdf2d to pmf2d
for i=1:divsx
    for j=1:divsy
        pmf2d(i,j)=-log(pdf2d(i,j));
    end
end


% create axis values

for i=1:divsx
    x_vals(i)=(Xmin+stepsize*i);
end

for i=1:divsy
    y_vals(i)=(Ymin+stepsize*i);
end

colstr1=num2str(compmat(1,1));
colstr2=num2str(compmat(1,2));
szx=size(x_vals);
szy=size(y_vals);
szp=size(pmf2d);


figure (1)
h=surf(y_vals,x_vals,pmf2d);
title('xxxxxx','FontWeight','bold')
set(h,'EdgeColor','none')
axis([Ymin  Ymax Xmin  Xmax]);
xlabel('xxxxxx', 'Fontsize', 8);
Ylabel('xxxxxx', 'Fontsize', 8);
```

2. Backbone Dihedral Angle ψ MATLAB Code:

```
clear all;
close all;

% file names:
filename='xxxxxxxx';


% Constants;
% ---------
Average=10;  % How many points you want to average (moving average)
N=5;         % How many dihedral psi angle you want to calculate
R=66;        % The row that you want readfile to start with
C=0;         % The coluomn that you want readfile to start with

% For energy plots:
%-----------------
Xmin= -180;
Xmax= 180;
stepsize=0.2;
```

```
% load data for 1st file:
dat=dlmread([filename '.csv'], '\t',R,C);

% what the size of my matrix
sz=size(dat);
sz(1);
moving=sz(1)-Average+1;


% The calculation of the dihedral angle:
% --------------------------------------

for i=1:sz(1);
    j=1;
    p=2;
    for L=1:1:N;

        xba=dat(i,p+3)-dat(i,p);
        yba=dat(i,p+4)-dat(i,p+1);
        zba=dat(i,p+5)-dat(i,p+2);

        xcb=dat(i,p+6)-dat(i,p+3);
        ycb=dat(i,p+7)-dat(i,p+4);
        zcb=dat(i,p+8)-dat(i,p+5);

        xdc=dat(i,p+9)-dat(i,p+6);
        ydc=dat(i,p+10)-dat(i,p+7);
        zdc=dat(i,p+11)-dat(i,p+8);

        xt=yba*zcb-ycb*zba;
        yt=zba*xcb-zcb*xba;
        zt=xba*ycb-xcb*yba;

        xu=ycb*zdc-ydc*zcb;
        yu=zcb*xdc-zdc*xcb;
        zu=xcb*ydc-xdc*ycb;

        xtu=yt*zu-yu*zt;
        ytu=zt*xu-zu*xt;
        ztu=xt*yu-xu*yt;

        rt2=xt^2+yt^2+zt^2;
        ru2=xu^2+yu^2+zu^2;
        rtru=sqrt(rt2*ru2);

        rcb=sqrt(xcb^2+ycb^2+zcb^2);

        sign=(xcb*xtu+ycb*ytu+zcb*ztu)/(rcb*rtru);

        psi(i,j)=(sign/abs(sign))*180*acos((xt*xu+yt*yu+zt*zu)/rtru)/pi;

        j=j+1;
        p=p+9;

    end
end
```

```
psiave=zeros(moving,N);

if Average>1;
   for L=1:1:N;
       for i=1:moving;
                for c=0:1:Average-1;
                    psiave(i,L)=psiave(i,L)+psi(i+c,L);
                end
            psiave(i,L)=psiave(i,L)/Average;
       end

   end
end



% the size of my matrix after doing the average:
szd=size(psi);
szdave=size(psiave);



divsx=(-Xmin+Xmax)/stepsize;


hist=zeros(divsx,N);


for u=1:1:N;

    tot=0;
    % initialize incidence counter
    for n=1:moving

    % evaluate dat1; data in column specified by first entry of 'compmat'
                psiave(n,u);
                x=round((psiave(n,u)-Xmin)/stepsize);

    % update histogram if within limits

        if ((x>0)&&(x<divsx))
                    hist(x,u)=hist(x,u)+1;
                    tot=tot+1;
        end

    end

end

pdf2d=hist/(tot-1);

% convert pdf2d to pmf2d
for i=1:divsx
    for j=1:N
         pmf2d(i,j)=-log(pdf2d(i,j));
    end
end

B=[1 1.9999 2 2.9999 3 3.9999 4 4.9999 5 5.9999];
```

```
for i=1:divsx
c=1;
    for j=1:N;
        pmf2B(i,c)=pmf2d(i,j);
        pmf2B(i,c+1)=pmf2d(i,j);
        c=c+2;
    end
end


% create axis values
for i=1:divsx
    x_val(i)=Xmin+stepsize*i;
end

pmf2B=transpose(pmf2B);
B=transpose(B);

figure (1);
h=surf(x_val,B, pmf2B);
title('xxxxxx','Fontweight','bold');
set(h,'EdgeColor','none')
axis([Xmin  Xmax 1 N+1]);
xlabel('xxxxxxxxxxxx','FontSize',8);
ylabel('xxxxxxxxxxxx','FontSize',8);
```

3. Hydrogen Donor-Acceptor Pairs MATLAB Code:

```
clear all;
close all;

% file names:
filename='xxxxxxxxxx';


% Constants;
% ---------
N=5;          % How many hydrogen donor acceptor pairs (residues) you want to
consider
R=88;         % The row that you want readfile to start with
C=1;          % The coluomn that you want readfile to start with
ymin = 0;
ymax = 1;
xmin=0;
xmax=7;

% load data for 1st file:
dat=dlmread([filename '.csv'],'\t', R,C);

sz=size(dat);

sz(1);

T=4;   %the possible number of pairs with each residue
Htype=zeros(N,2*T);
```

```
p=1;
ss=0;

% The calculation of the hydrogen donor acceptor pairs:
% ----------------------------------------------------

for L=1:1:N;

    for i=1:sz(1);
        kk=0;
        v=0;
        m=zeros(T+4);

        for j=1:1:T;

        x1=dat(i,p)-dat(i,15+v+p);
        x2=dat(i,42+v+p)-dat(i,15+v+p);

        y1=dat(i,p+1)-dat(i,16+v+p);
        y2=dat(i,43+v+p)-dat(i,16+v+p);

        z1=dat(i,p+2)-dat(i,17+v+p);
        z2=dat(i,44+v+p)-dat(i,17+v+p);

        A=sqrt(x1^2+y1^2+z1^2);
        B=sqrt(x2^2+y2^2+z2^2);

        AB=A*B;
        AdotB=x1*x2+y1*y2+z1*z2;
        Hangle=180*acos(AdotB/AB)/pi;
        Hdis=10*A;


            if ( (Hangle<30) && (Hdis<3.5) );
                m(j)=1;
            end
            kk=kk+m(j);
            v=v+3;
        end
        m;
        kk;
        if kk==0;
           Htype(L,T+1)=Htype(L,T+1)+1;
        elseif kk==1;
            for j=1:1:T;
            Htype(L,j)=Htype(L,j)+m(j);
            end
        else
            for j=1:1:T;
            if ((m(j)==1) && (m(j+1)==1));
               Htype(L,j+T+1)=Htype(L,j+T+1)+1;
            end
            end
        end

    end
    p=p+3;
end
```

```
for i=1:N;
    Htype1(i,1)=Htype(i,2);
    Htype1(i,2)=Htype(i,3);
    Htype1(i,3)=Htype(i,4);
    Htype1(i,4)=Htype(i,5);
    Htype1(i,5)=Htype(i,7);
    Htype1(i,6)=Htype(i,8);
end

Htype1=transpose(Htype1/sz(1));

Figure (1)
h=bar(Htype1);
title('xxxxxxxxxxx','FontWeight','bold');
axis([xmin xmax ymin ymax]);
xlabel('xxxxxxxxxx','FontSize',8);
ylabel('xxxxxxxxxx','FontSize',8);
```

4. Salt Bridge's Calculation MATLAB Codes:

a. Energy landscape plots:

```
clear all;
close all;

% file name;
filename1='xxxxxxxxxxx';



% Constants;
% ---------
Average=15;  % How many points you want to average (moving average)
N=2;         % How many distances you want to calculate
R=36;        % The row that you want readfile to start with
C=0;         % The coluomn that you want readfile to start with


% number of columns to compare
numcomp=1;
compmat=[1 2];

% For energy plots:
%-----------------
Xmin= 0;
Xmax= 3;
Ymin= 0;
Ymax= 3;
stepsize=0.01;



% load data for 1st file:
```

```
dat=dlmread([filename '.csv'], '\t',R,C);

% what the size of my matrix
sz=size(dat);
sz(1);
moving=sz(1)-Average+1;


% The calculation of the distance:
% --------------------------------
for i=1:sz(1);
    p=2;
    for L=1:1:N;
    x=dat(i,p)-dat(i,p+3);
    y=dat(i,p+1)-dat(i,p+4);
    z=dat(i,p+2)-dat(i,p+5);
    D(i,L)=sqrt(x^2+y^2+z^2);
    p=p+6;
    end
end

Dave=zeros(moving,N);

if Average>1;
   for L=1:1:N;
       for i=1:moving;
                for c=0:1:Average-1;
                    Dave(i,L)=Dave(i,L)+D(i+c,L);
                end
            Dave(i,L)=Dave(i,L)/Average;
       end

   end
end

% the size of my matrix after doing the average:
szd=size(D);
szdave=size(Dave);


divsx=(-Xmin+Xmax)/stepsize;
divsy=(-Ymin+Ymax)/stepsize;

for i=1:divsx
    for j=1:divsy
        hist(i,j)=0;
    end
end

tot=0;

    % loop through images
    for n=1:moving

   % evaluate dat1; data in column specified by first entry of 'compmat'

                x=round((Dave(n,1)-Xmin)/stepsize);

   % evaluate dat2; data in column specified by second entry of 'compmat'
```

```
                y=round((Dave(n,2)-Ymin)/stepsize);

   % update histogram if within limits

        if ((x>0)&&(x<divsx))&&((y>0)&&(y<divsy))
                    hist(x,y)=hist(x,y)+1;
                    tot=tot+1;
        end

    end

% end loop over distances

pdf2d=hist/(tot-1);

% convert pdf2d to pmf2d
for i=1:divsx
    for j=1:divsy
        pmf2d(i,j)=-log(pdf2d(i,j));
    end
end

% create axis values

for i=1:divsx
    x_vals(i)=(Xmin+stepsize*i);
end

for i=1:divsy
    y_vals(i)=(Ymin+stepsize*i);
end

colstr1=num2str(compmat(1,1));
colstr2=num2str(compmat(1,2));
szx=size(x_vals);
szy=size(y_vals);
szp=size(pmf2d);

h=surf(y_vals,x_vals,pmf2d);
title('xxxxxxx','FontWeight','bold');
set(h,'EdgeColor','none');
axis([Ymin  Ymax Xmin  Xmax]);
xlabel('xxxxxxxxxxxxx', 'Fontsize', 8);
Ylabel('xxxxxxxxxxxxx', 'Fontsize', 8);
```

b. Cumulative probability plots:

```
clear all;
close all;

% file name;
filename='xxxxxxxxxxx';

% Constants;
% ---------
Average=10;  % How many points you want to average (moving average)
N=2;         % How many distance you want to calculate
```

```
R=30;         % The row that you want readfile to start with
C=0;          % The coluomn that you want readfile to start with
Xmin=0;
Xmax=3;
Ymin=0;
Ymax=1;
stepsize=0.01;

% load data for 1st file:
dat=dlmread([filename '.csv'], '\t',R,C);


sz=size(dat);
sz(1);
moving=sz(1)-Average+1;


% The calculation of the distance:
% --------------------------------

for i=1:sz(1);
    p=2;
    for L=1:1:N;
    x=dat(i,p)-dat(i,p+3);
    y=dat(i,p+1)-dat(i,p+4);
    z=dat(i,p+2)-dat(i,p+5);
    D(i,L)=sqrt(x^2+y^2+z^2);
    p=p+6;
    end
end

Dave=zeros(moving,N);

if Average>1;
   for L=1:1:N;
       for i=1:moving;
                for c=0:1:Average-1;
                    Dave(i,L)=Dave(i,L)+D(i+c,L);
                end
            Dave(i,L)=Dave(i,L)/Average;
       end

   end
end

% the size of my matrix after doing the average:
szd=size(D);
szdave=size(Dave);


divsx=(-Xmin+Xmax)/stepsize;


hist=zeros(divsx,N);

totp=0;
for u=1:1:N;

    tot=totp;
```

```
    % initialize incidence counter
    for n=1:moving

    % evaluate dat1; data in column specified by first entry of 'compmat'
                Dave(n,u);
                x=round((Dave(n,u)-Xmin)/stepsize);

    % update histogram if within limits

        if ((x>0)&&(x<divsx))
                    hist(x,u)=hist(x,u)+1;
                    tot=tot+1;
        end

    end

end
totp=tot;

for i=1:divsx
    x_vals(i)=Xmin+stepsize*i;
end


hist=hist/(tot-1);

szhist=size(hist);

cl=0;
bl=0;


for i=1:szhist(1);

    cl=cl+hist(i,1);
    bl=bl+hist(i,2);

    probhist(i,1)=cl;
    probhist(i,2)=bl;

end



plot(x_vals,probhist)
axis([Xmin Xmax Ymin Ymax]);
title('xxxxxxx','FontWeight','bold');
xlabel('xxxxxxx', 'Fontsize', 8);
ylabel('xxxxxxx', 'Fontsize', 8);
grid
```

5. H1/H4 Tail Interactions MATLAB Code:

```
clear all;
close all;

% file name;
filename='xxxxxxxxxxxxx';


% Constants;
% ---------
R=186;         % The row that you want readfile to start with
C=0;          % The coluomn that you want readfile to start with
NO=4;
Prob=0.1;
Xmin= -0.5;
stepsize=1;
N=2;
Ymax=1;


% load data
dat=dlmread([filename '.csv'], '\t',R,C);


sz=size(dat);

% The calculation of the distance:
% --------------------------------

p=2;
v=0;
j=1;
for kk=1:1:13;

    w=137;
    for L=1:1:11;

        for i=1:sz(1);

        x=dat(i,p)-dat(i,w);
        y=dat(i,p+1)-dat(i,w+1);
        z=dat(i,p+2)-dat(i,w+2);
        DNO(i,j)=10*sqrt(x^2+y^2+z^2);

        end
        j=j+1;
        w=w+3;
    end
    p=p+3;

end


p=41;
v=0;
```

```
j=1;
for kk=1:1:19;

    w=98;
    for L=1:1:13;

        for i=1:sz(1);

        x=dat(i,p)-dat(i,w);
        y=dat(i,p+1)-dat(i,w+1);
        z=dat(i,p+2)-dat(i,w+2);
        DON(i,j)=10*sqrt(x^2+y^2+z^2);

        end
        j=j+1;
        w=w+3;
    end
    p=p+3;

end

szDNO=size(DNO);
szDON=size(DON);

DNOt(1:szDNO(2))=0;
DONt(1:szDON(2))=0;


for j=1:szDNO(2);

      for i=1:sz(1);

          if DNO(i,j)<=NO;
              DNOProb(i,j)=1;
              DNOt(j)=DNOt(j)+1;
          else
              DNOProb(i,j)=0;
          end

      end
end

for j=1:szDON(2);

      for i=1:sz(1);

          if DON(i,j)<=NO;
              DONProb(i,j)=1;
              DONt(j)=DONt(j)+1;
          else
              DONProb(i,j)=0;
          end

      end
end

DONt=DONt/sz(1);
DNOt=DNOt/sz(1);
```

```
szNON=szDON(2)+szDNO(2);

jj=1;
for j=1:szNON;
    if j<=szDNO(2);
        if DNOt(j)>=Prob;
            Final(jj,1)=j;
            Final(jj,2)=DNOt(j);
            jj=jj+1;
        end
    else
        if DONt(j-szDNO(2))>=Prob;
            Final(jj,1)=j;
            Final(jj,2)=DONt(j-szDNO(2));
            jj=jj+1;
        end
    end
end
Xmax=0;

for i=1:sz(1);
    interact=0;
    for j=1:szNON;
        if j<=szDNO(2);
            if DNOProb(i,j)==1;
                interact=interact+1;
            end
        else
            if DONProb(i,j-szDNO(2))==1;
                interact=interact+1;
            end
        end
    end
        inter(i,1)=interact;
        if Xmax<interact;
            Xmax=interact;
        end

end


Xmax=Xmax+0.5;

divsx=(-Xmin+Xmax)/stepsize;

hist=zeros(divsx,N);

for u=1:1:N;

% initialize incidence counter
tot=0;

    for n=1:sz(1);

      % evaluate dat1; data in column specified by first entry of 'compmat'
                inter(n,u);
                x=round((inter(n,u)-Xmin)/stepsize);

       % update histogram if within limits
```

```
        if ((x>0)&&(x<divsx))
                    hist(x,u)=hist(x,u)+1;
                    tot=tot+1;
        end
    end
    hist(:,u)=hist(:,u)/tot;

end

bar(0:Xmax, hist)
axis([Xmin Xmax 0 Ymax]);
ylabel('xxxxxxx');
xlabel('xxxxxxx');
```

6. H1/H4 Tail Position MATLAB Code:

```
clear all;
close all;

% file name;
filename='xxxxxxxx';

% Constants;
% ---------
Average=15;  % How many points you want to average (moving average)
N=2;         % How many torsion angle you want to calculate
R=42;        % The row that you want readfile to start with
C=0;         % The coluomn that you want readfile to start with

compmat=[1 2];


% number of columns to compare
numcomp=1;

% For energy plots:
%-----------------
Xmin= -180;
Xmax= 180;
Ymin= -180;
Ymax= 180;
stepsize=1;


 % load data for 1st file:
dat=dlmread([filename '.csv'], '\t',R,C);

% what the size of my matrix
sz=size(dat);
sz(1);
moving=sz(1)-Average+1;
```

```
% The calculation of the torsion angle:
% -----------------------------------
i=0;
p=2;
for i=1:sz(1);
    j=1;
    p=2;
    for L=1:1:N;

        xba=dat(i,p+3)-dat(i,p);
        yba=dat(i,p+4)-dat(i,p+1);
        zba=dat(i,p+5)-dat(i,p+2);

        xcb=dat(i,p+6)-dat(i,p+3);
        ycb=dat(i,p+7)-dat(i,p+4);
        zcb=dat(i,p+8)-dat(i,p+5);

        xdc=dat(i,p+9)-dat(i,p+6);
        ydc=dat(i,p+10)-dat(i,p+7);
        zdc=dat(i,p+11)-dat(i,p+8);

        xt=yba*zcb-ycb*zba;
        yt=zba*xcb-zcb*xba;
        zt=xba*ycb-xcb*yba;

        xu=ycb*zdc-ydc*zcb;
        yu=zcb*xdc-zdc*xcb;
        zu=xcb*ydc-xdc*ycb;

        xtu=yt*zu-yu*zt;
        ytu=zt*xu-zu*xt;
        ztu=xt*yu-xu*yt;

        rt2=xt^2+yt^2+zt^2;
        ru2=xu^2+yu^2+zu^2;
        rtru=sqrt(rt2*ru2);

        rcb=sqrt(xcb^2+ycb^2+zcb^2);

        sign=(xcb*xtu+ycb*ytu+zcb*ztu)/(rcb*rtru);

        psi(i,j)=(sign/abs(sign))*180*acos((xt*xu+yt*yu+zt*zu)/rtru)/pi;

        j=j+1;
        p=p+12;

    end
end


divsx=(-Xmin+Xmax)/stepsize;
divsy=(-Ymin+Ymax)/stepsize;

for i=1:divsx
    for j=1:divsy
        hist(i,j)=0;

    end
end
```

```
tot=0;

for p=1:numcomp(1)

    % loop through images
    for n=1:sz(1)

    % evaluate dat1; data in column specified by first entry of 'compmat'
        psi(n,compmat(p,1))
                x=round((psi(n,compmat(p,1))-Xmin)/stepsize);

    % evaluate dat2; data in column specified by second entry of 'compmat'
                y=round((psi(n,compmat(p,2))-Ymin)/stepsize);

    % update histogram if within limits

        if ((x>0)&&(x<divsx))&&((y>0)&&(y<divsy))
                    hist(x,y)=hist(x,y)+1;
                    tot=tot+1;
        end

    end



% end loop over distances
end

psi;
hist;
pdf2d=hist/tot;

% convert pdf2d to pmf2d
for i=1:divsx
    for j=1:divsy
        pmf2d(i,j)=-log(pdf2d(i,j));
    end
end


% create axis values
for i=1:divsx
    x_vals(i)=Xmin+stepsize*i;
end

for i=1:divsy
    y_vals(i)=Ymin+stepsize*i;
end

colstr1=num2str(compmat(1,1));
colstr2=num2str(compmat(1,2));
szx=size(x_vals);
szy=size(y_vals);
szp=size(pmf2d);


h=surf(y_vals,x_vals,pmf2d);
title('xxxxxxx','FontWeight','bold')
set(h,'EdgeColor','none')
```

```
axis([Ymin  Ymax Xmin  Xmax]);
xlabel('xxxxxxxxxx', 'Fontsize', 9);
Ylabel('xxxxxxxxxx', 'Fontsize', 9);
```

Appendix D. H1/H4 Tail Interaction Tables

Equilibrium Simulations

1. Equilibrium simulations for augmented FAT/paxillin complex (with H4 tail and P1/P2 constrained):

Table D-1: Electrostatic interactions found between H1/H4 tail that have a probability greater than 10% of 20 ns simulation time long. These runs belong to the equlibrion simulation of the FAT/paxillin complex (with H4 tail and P1/P2 constrained).

Run#1			**Run#2**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
O: 915	NE2: 1052	0.2215	There is no interaction has probability greater than 10%		
O: 916	NE2: 1052	0.2496			
OD1: 916	NE2: 1052	0.1651			
Run#3			**Run#4**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 918	O: 1047	0.5518	N: 916	OD1: 1048	0.1797
O: 916	N: 1047	0.3914	N: 918	O: 1048	0.1397
O: 916	N: 1050	0.1285	N: 918	O: 1049	0.5158
O: 918	N: 1049	0.3325	O: 910	NZ: 1044	0.1628
CG: 918	NE2: 1048	0.1849	O: 916	N: 1049	0.1699
			O: 916	N: 1050	0.2223
			O: 916	CZ: 1050	0.1936
			CG: 918	NE2: 1052	0.119

2. Equilibrium simulation for augmented FAT/paxillin with H4 tail and P1 constrained (without P2):

Table D-2: Electrostatic interactions found between H1/H4 tail that have a probability greater than 10% of 20 ns simulation time long. These runs belong to the equlibrion simulation of the augmented FAT/paxillin complex (with H4 tail and P1 constrained).

Run#1			**Run#2**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 916	O: 1050	0.1127	OD1: 916	N: 1043	0.2407
N: 918	O: 1048	0.8887			
N: 919	O: 1048	0.1012			
O: 915	N: 1052	0.125			
O: 915	NE2: 1052	0.1143			
O: 916	N: 1050	0.9277			
O: 919	NE2: 1048	0.1262			
CG: 918	NE2: 1048	0.202			
CG: 918	NE2: 1052	0.2056			
OG: 920	NE2: 1048	0.1136			
Run#3			**Run#4**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
O: 916	CZ: 1050	0.1267	N: 916	O: 1048	0.417
OG1: 914	NZ: 1044	0.1241	N: 916	O: 1050	0.129
OD1: 916	N: 1044	0.1891	N: 917	O: 1048	0.1771
OD1: 916	NZ: 1044	0.1826	N: 918	O: 1048	0.3751
			N: 918	OD1: 1048	0.5523
			ND2: 916	O: 1050	0.2855
			O: 916	N: 1049	0.2392
			O: 916	N: 1050	0.8814
			O: 917	NE2: 1052	0.1664
			CG: 918	NE2: 1052	0.1883

Loaded Simulations

1. Axial load simulations for augmented FAT/paxillin complex (with H4 tail and P1/P2 constrained):

Typical behavior:

Table D-3: Electrostatic interactions found between H1/H4 tail that have a probability greater than 10% of 20 ns simulation time long. These runs belong to the axial load simulations of the augmented FAT/paxillin complex (with H4 tail and P1 constrained). They represent the typical behavior of H1.

Seed#1: Run#1			**Seed#1: Run#2**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 914	C: 1052	0.1959	N: 915	O: 1048	0.8813
N: 916	O: 1050	0.879	N: 917	O: 1045	0.5673
N: 918	O: 1048	0.8718	N: 917	O: 1046	0.1737
N: 920	O: 1046	0.254	O: 913	N: 1050	0.9012
CZ: 919	O: 1046	0.119	O: 915	N: 1047	0.5108
O: 914	N: 1052	0.6747	O: 915	N: 1048	0.7827
O: 916	N: 1050	0.9416	OG: 910	NE2: 1052	0.134
O: 918	N: 1047	0.2499	OD1: 916	N: 1047	0.6155
O: 918	N: 1048	0.6659			
CG: 918	NE2: 1052	0.1512			
Seed#2: Run#1			**Seed#3: Run#1**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 917	C: 1052	0.2389	N: 916	O: 1049	0.5874
N: 918	OD1: 1048	0.1182	N: 916	O: 1050	0.2203
N: 920	O: 1048	0.2079	N: 918	O: 1047	0.6823
ND2: 916	C: 1052	0.5857	N: 920	O: 1045	0.392
CZ: 919	O: 1049	0.1632	CZ: 919	O: 1043	0.2282
O: 915	N: 1052	0.1459	CZ: 919	O: 1046	0.1877
O: 917	N: 1052	0.408	O: 914	N: 1052	0.1997
O: 918	N: 1050	0.1058	O: 916	N: 1049	0.9249
OD1: 916	N: 1052	0.1746	O: 916	N: 1050	0.2801
			O: 918	N: 1047	0.629

Table D-3: Continue ..

Seed#3: Run#2			**Seed#4: Run#1**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 916	O: 1046	0.161	N: 916	O: 1047	0.1739
N: 917	O: 1046	0.1539	N: 916	OD1: 1048	0.1752
N: 917	O: 1049	0.3165	N: 917	O: 1049	0.1685
N: 918	O: 1046	0.347	N: 918	O: 1049	0.3927
N: 918	O: 1048	0.4454	N: 919	O: 1049	0.2362
N: 918	O: 1049	0.4482	N: 920	O: 1049	0.286
ND2: 916	O: 1048	0.2286	ND2: 916	O: 1049	0.1042
ND2: 916	O: 1049	0.1174	ND2: 921	C: 1052	0.2813
CZ: 919	O: 1043	0.1523	O: 914	NE2: 1048	0.1768
O: 916	N: 1048	0.836	O: 916	N: 1049	0.4676
O: 916	N: 1049	0.2705	O: 916	NE2: 1048	0.1534
O: 918	N: 1046	0.3182	O: 918	N: 1049	0.3347
O: 918	NE2: 1048	0.2907	OD1 921	N: 1052	0.3661
O: 921	NE2: 1048	0.3052			
OD1: 916	CZ: 1050	0.1412			
CG: 918	NE2: 1048	0.1664			
Seed#4: Run#2			**Seed#5: Run#2**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 916	O: 1047	0.1148	N: 920	OD1: 1048	0.1212
N: 918	O: 1049	0.2529			
N: 920	O: 1050	0.4338			
N: 921	C: 1052	0.1649			
CZ: 919	O: 1043	0.171			
ND2: 921	C: 1052	0.2518			
O: 916	N: 1049	0.2106			
O: 918	N: 1050	0.4007			
O: 919	N: 1052	0.1217			
OG: 920	N: 1052	0.1039			

Atypical behavior:

Table D-4: Electrostatic interactions found between H1/H4 tail that have a probability greater than 10% of 20 ns simulation time long. These runs belong to the axial load simulations of the augmented FAT/paxillin complex (with H4 tail and P1 constrained). They represent the atypical behavior of H1.

Seed#1: Run#1			**Seed#2: Run#2**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 916	O: 1050	0.406	There is no interaction has probability greater than 10%		
N: 918	O: 1048	0.9292			
ND2: 916	O: 1050	0.1429			
CZ: 919	O: 1046	0.1169			
O: 914	N: 1052	0.2661			
O: 915	N: 1052	0.2436			
O: 916	N: 1050	0.8778			
O: 918	N: 1048	0.8852			
CG: 918	NE2: 1052	0.5813			

2. Perpendicular load simulations for augmented FAT/paxillin complex (with H4 tail and P1 constrained):

Typical behavior:

Table D-5: Electrostatic interactions found between H1/H4 tail that have a probability greater than 10% of 20 ns simulation time long. These runs belong to the perpendicular load simulations of the augmented FAT/paxillin complex (with H4 tail and P1 constrained). They represent the typical behavior of H1.

Seed#1: Run#2			**Seed#2: Run#2**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 920	O: 1051	0.2253	N: 915	C: 1052	0.1028
O: 920	NE2: 1052	0.1299	N: 916	O: 1050	0.2593
O: 921	CZ: 1050	0.1732	N: 918	O: 1048	0.9866
OG: 920	CZ: 1050	0.1915	N: 920	O: 1046	0.3248
			N: 920	OD1: 1048	0.1113
			CZ: 919	O: 1043	0.3015
			CZ: 919	O: 1044	0.1023
			O: 914	N: 1052	0.1413
			O: 915	N: 1052	0.4923
			O: 916	N: 1050	0.9523
			O: 918	N: 1048	0.6669
			O: 919	NE2: 1048	0.1396
			OG1: 914	N: 1052	0.1708
			CG: 918	NE2: 1048	0.1329
			CG: 918	NE2: 1052	0.483
			OG: 920	NE2: 1048	0.1679
			OD1 921	NE2: 1048	0.1015
Seed#3: Run#1			**Seed#3: Run#2**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 914	C: 1052	0.1678	N: 918	O: 1049	0.1209
N: 916	O: 1050	0.4776	ND2: 921	OD1: 1048	0.1062
N: 918	O: 1048	0.9859			
N: 920	O: 1046	0.124			
CZ: 919	O: 1043	0.1696			
CZ: 919	O: 1044	0.2113			
CZ: 919	O: 1046	0.1067			
O: 914	N: 1052	0.3904			
O: 915	N: 1052	0.2933			
O: 916	N: 1050	0.9705			
O: 918	N: 1048	0.734			
O: 919	NE2: 1048	0.1337			
OG1: 914	N: 1052	0.1021			
CG: 918	NE2: 1048	0.1492			
CG: 918	NE2: 1052	0.3846			
OG: 920	NE2: 1048	0.1024			

Table D-5: Continue ..

Seed#4: Run#1			**Seed#4: Run#2**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 914	C: 1052	0.1146	N: 914	C: 1052	0.1578
N: 916	O: 1050	0.8907	N: 916	O: 1050	0.7926
N: 918	O: 1048	0.9765	N: 918	O: 1048	0.9798
N: 920	O: 1045	0.5482	N: 920	O: 1046	0.4227
ND2: 916	O: 1050	0.1313	O: 914	N: 1052	0.601
CZ: 919	O: 1046	0.1936	O: 916	N: 1050	0.9861
O: 914	N: 1052	0.6374	O: 918	N: 1048	0.6895
O: 916	N: 1050	0.9942	CG: 918	NE2: 1052	0.1819
O: 918	N: 1047	0.5003			
O: 918	N: 1048	0.7791			
O: 920	N: 1046	0.2738			
OD1: 916	NE2: 1052	0.1129			
CG: 918	NE2: 1048	0.1003			
CG: 918	NE2: 1052	0.1111			
OG: 920	NE2: 1048	0.1088			
Seed#5: Run#1			**Seed#5: Run#2**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 916	C: 1052	0.3008	N: 920	O: 1049	0.6024
N: 918	O: 1050	0.9319	CZ: 919	O: 1051	0.1285
N: 920	O: 1048	0.8746	O: 918	N: 1049	0.1382
O: 916	N: 1052	0.9408	CG: 918	N: 1049	0.1255
O: 918	N: 1050	0.8821	CG: 918	NE2: 1048	0.1572
O: 920	NE2: 1048	0.6003	OG: 920	N: 1049	0.1248
CG: 918	NE2: 1052	0.389	OG: 920	NE2: 1048	0.2407
			OD1 921	CZ: 1050	0.1402
Seed#6: Run#1					
Electrostatic Interaction [atoms: residue #]		Probability			
H1 tail	H4 tail				
There is no interaction has probability greater than 10%					

Atypical behavior:

Table D-6: Electrostatic interactions found between H1/H4 tail that have a probability greater than 10% of 20 ns simulation time long. These runs belong to the perpendicular load simulations of the augmented FAT/paxillin complex (with H4 tail and P1 constrained). They represent the atypical behavior of H1.

Seed#1: Run#1			**Seed#2: Run#1**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 920	O: 1051	0.2606	N: 914	C: 1052	0.2713
O: 918	CZ: 1050	0.1322	N: 916	O: 1050	0.8453
OG: 920	CZ: 1050	0.1113	N: 918	O: 1048	0.9947
			N: 920	O: 1045	0.2004
			N: 920	O: 1046	0.308
			CZ: 919	O: 1043	0.2924
			CZ: 919	O: 1044	0.1211
			CZ: 919	O: 1046	0.1833
			O: 914	N: 1052	0.743
			O: 916	N: 1050	0.9936
			O: 918	N: 1047	0.2627
			O: 918	N: 1048	0.7875
			CG: 918	NE2: 1048	0.1038
			CG: 918	NE2: 1052	0.3026
			OG: 920	NE2: 1048	0.1165

Seed#6: Run#2		
Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail	
`There is no interaction has probability greater than 10%		

Repeatability of atypical behavior:

Table D-7: Electrostatic interactions found between H1/H4 tail that have a probability greater than 10% of 20 ns simulation time long. These runs belong to the perpendicular load simulations of the augmented FAT/paxillin complex (with H4 tail and P1 constrained). They represent the repeatability of atypical behavior of H1.

Seed#1: Run#3			**Seed#1: Run#4**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 917	C: 1052	0.2033	N: 914	O: 1050	0.2119
N: 918	O: 1049	0.1513	N: 915	O: 1048	0.2585
N: 918	C: 1052	0.128	N: 916	O: 1048	0.5311
ND2: 916	C: 1052	0.2254	N: 918	O: 1046	0.4265
			ND2: 916	O: 1046	0.1199
			O: 913	N: 1050	0.2539
			O: 913	NE2: 1052	0.1054
			O: 914	N: 1050	0.2598
			O: 914	CZ: 1050	0.1424
			O: 915	N: 1048	0.2192
			O: 916	N: 1047	0.1185
			O: 916	N: 1048	0.6149
			CG: 918	NE2: 1048	0.1683
Seed#1: Run#5			**Seed#1: Run#6**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
There is no interaction has probability greater than 10%			N: 915	O: 1050	0.7948
			N: 917	O: 1048	0.8267
			ND2: 916	O: 1046	0.1007
			ND2: 916	O: 1048	0.1248
			CZ: 919	O: 1043	0.1396
			CZ: 919	O: 1046	0.2275
			CZ: 919	O: 1047	0.1311
			O: 913	N: 1052	0.4703
			O: 915	N: 1050	0.9408
			O: 917	N: 1048	0.1711
			O: 918	N: 1047	0.1105
			OD1: 916	N: 1048	0.2052
Seed#1: Run#7			**Seed#1: Run#8**		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 920	O: 1051	0.1002	N: 918	OD1: 1048	0.2293
O: 921	CZ: 1050	0.1162	O: 916	NE2: 1048	0.4291
OG: 920	CZ: 1050	0.1466	O: 918	N: 1048	0.7627
			O: 918	N: 1049	0.7857
			O: 920	N: 1043	0.521
			CG: 918	N: 1048	0.2887
			CG: 918	NE2: 1048	0.4074

Table D-7: Continue ..

Seed#1: Run#9			Seed#1: Run#10		
Electrostatic Interaction [atoms: residue #]		Probability	Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail		H1 tail	H4 tail	
N: 914	C: 1052	0.1813	CZ: 919	O: 1043	0.1223
N: 916	O: 1050	0.7156	O: 918	N: 1048	0.1673
N: 917	O: 1050	0.1112			
N: 918	O: 1048	0.7587			
N: 920	O: 1046	0.1367			
CZ: 919	O: 1043	0.3087			
CZ: 919	O: 1046	0.2145			
O: 914	N: 1052	0.4565			
O: 916	N: 1050	0.8193			
O: 918	N: 1048	0.6148			
OD1: 916	N: 1052	0.1595			
CG: 918	NE2: 1052	0.2529			
OG: 920	NE2: 1048	0.1034			

Seed#1: Run#11		
Electrostatic Interaction [atoms: residue #]		Probability
H1 tail	H4 tail	
There is no interaction has probability greater than 10%		

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